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CRYSTAL STRUCTURE OF THE BTK KINASE DOMAIN

This application claims priority to United States Provisional Application Serial No. 60/339,206, filed December 7, 2001 and United States Provisional Application Serial No. 60/312,597, filed August 15, 2001.

Field of the Invention

This invention relates to the crystal structure of the Bruton's Tyrosine Kinase (BTK) kinase domain (KD).

Background of the Invention

Bruton's tyrosine kinase (BTK), a member of the BTK/TEC family of cytoplasmic protein tyrosine kinases (PTKs), is intimately involved in signal transduction pathways regulating survival, activation, proliferation, and differentiation of B-lineage lymphoid cells (30, 34, 50, 61, 64). Signal transduction pathways are initiated by the binding of a variety of extracellular ligands, such as antigens, to cell surface receptors (30). Following ligation of the B-cell antigen receptor, BTK activation by the concerted actions of the PTKs LYN and SYK is required for induction of phospholipase C-γ2 mediated calcium mobilization (30). Mutations in the human *BTK* gene are the cause of X-linked agammaglobulinemia (XLA), a male immune deficiency disorder characterized by a lack of mature, immunoglobulin-producing, peripheral B-cells (58, 65). In mice, mutations in the *btk* gene have been identified as the cause of murine X-linked immune deficiency (51).

BTK is a dual-function regulator of apoptosis, in that it promotes radiation-induced apoptosis, but inhibits Fas-activated apoptosis in B-cells (59, 61). BTK promotes apoptosis when B-cells are exposed to reactive oxygen intermediates, partly by down-regulating the anti-apoptotic activity of STAT3 transcription factor. In contrast, BTK inhibits apoptosis when it associates with the death receptor Fas and impairs its interaction with FADD. The interaction between Fas and FADD is essential for the recruitment and activation of FLICE by Fas during the apoptotic signal, thereby preventing the assembly of a proapoptotic death-inducing signaling complex (DISC) after Fas-ligation.

The amino acid sequence of BTK has been determined for human and mouse and functional domains have been assigned (5, 48, 58). The N-terminal region contains a pleckstrin homology (PH) domain followed by a proline-rich TEC homology (TH) domain. The PH domain is the site of both activation (by phosphatidylinositol phosphates and G-protein $\beta\gamma$ subunits) and inhibition (by protein kinase C) (58). The remaining portion of BTK contains SRC homology (SH) domains SH3, SH2, and a C-terminal kinase domain, also known as the SH1 domain. The SH2 domain mediates binding to tyrosine-phosphorylated peptide motifs on other molecules, while the SH3 domain mediates binding to proline-rich motifs on other molecules. Mutations in the SH1 domain, SH2 domain, and the PH domain of human BTK have been found to cause maturational blocks at early stages of B-cell ontogeny leading to XLA (67). BTK-deficient mice generated by introducing PH domain or SH1 domain mutations into the BTK gene of embryonic stem cells exhibit defective B-cell development and function (25). The crystal structure of the PH domain has been determined and has contributed to a structural understanding of how point mutations of the PH domain can inactivate BTK and cause XLA (21). However, the crystal structure of the kinase domain has not been resolved.

The BTK polypeptide (SEQ ID NO: 1 or SEQ ID NO: 2) includes two regulatory tyrosine residues, Y223 and Y551, which participate in kinase activation (52). An SRC family PTK, such as LYN, initially activates BTK through transphosphorylation of Y551 (SEQ ID NO: 1 or SEQ ID NO: 2) on the presumed "activation loop" (A-loop) of the kinase domain. This activation, in turn, stimulates autophosphorylation of the Y223 (SEQ ID NO: 1 or SEQ ID NO: 2) residue within the SH3 domain ligand-binding site (43, 44, 46, 49, 50, 52, 68). Phosphorylation of Y223 may function to disrupt an intramolecular TH-SH3 domain interaction, allowing the BTK TH domain to bind SH3 domains of SRC family PTKs, and the BTK PH domain to bind a proline-rich region of CBL (2, 30, 33). In other members of the PTK and PSK families, the A-loop serves as a negative regulator of kinase activity by blocking access of substrates to the ATP and substrate peptide binding sites that lie in the catalytic cleft of the kinase domain (20, 23). In some members, including apo-IRK, the catalytic site is sterically blocked by amino residues in the A loop acting as a substrate peptide mimic (18, 19).

The mechanism by which phosphorylation of Y551 (SEQ ID NO: 1 or SEQ ID NO: 2) brings about conformational changes in the kinase domain as well as kinase activation has not been elucidated. This structural question begs the illustration of a solved crystal structure. Furthermore the dimensions, conformation and binding properties of the substrate binding sites for ATP and substrates within the kinase domain are not known. Molecular interaction with BTK inducing phosphorylation of Y551 (SEQ ID NO: 1 or SEQ ID NO: 2) within the kinase domain and initial activation of BTK is not understood. Similarly, there is no structural understanding of how XLA is caused by various mutations within the BTK kinase domain.

In addition to providing answers to the above questions, determining the crystal structure of the kinase domain of BTK is needed, for a host of applied purposes, such as: assays for BTK-ligand interaction and function, modeling the structure-function relationship of BTK and other molecules, diagnostic assays for mutation-induced pathologies, and rational design of agents useful in modulating BTK activity.

Modulators of BTK are useful, for example, to promote or induce apoptosis in a BTK-expressing cell by inhibiting or preventing the action of BTK, to treat a disease (pathologic condition) where BTK is implicated and inhibition of its action is desired (e.g. cancer, such as leukemia or lymphoma), and to lower the resistance of a BTK expressing cell to drug therapy by inhibiting or preventing the action of BTK.

Summary of the Invention

The X-ray crystal structure of the kinase domain of BTK (BTK-KD) has now been determined by multiple isomorphous replacement. Coordinates of the crystal structure are listed in Table 4 ~~5~~.

The invention provides the crystal structure of the BTK-KD, as well as use of the crystal structure to model BTK activity. This use of the structure includes modeling the interaction of ligands with the BTK-KD; activation and inhibition of BTK; and the rational design of modulators of BTK activity. For example, these modulators include ligands that interact with BTK-KD and modulate BTK activities, such as the survival, activation, proliferation, and differentiation of B-lineage lymphoid cells.

Brief Description of Figures

Figure 1 is a ribbon representation of the dimeric crystal structure of the BTK-KD (amino acids 397 to 659 of SEQ ID NO:2). Resolution of the BTK-KD (amino acids 397 to 659 of SEQ ID NO:2) crystal structure revealed several structural features of the kinase domain. The N-terminal lobe 10 (amino acid residues I397-E475 of SEQ ID NO:2) contains five strands of anti-parallel β sheets (β1- β5) and one α-helix (αC). The C-terminal lobe 12 (amino acid residues N479-S659 of SEQ ID NO:2) contains a 4-helix bundle flanked by a short antiparallel β sheet and four additional helices. The N- and C-lobes are connected by a linker region 14 (amino acid residues E475-N479 of SEQ ID NO:2) and form a cleft 16 at the ATP binding site.

Figure 2 is a 2Fo-Fc electron density map (contoured at 1.0 σ) surrounding the R544, E445, and Y551 residues of the BTK-KD (amino acids 397 to 659 of SEQ ID NO:2) crystal, shown in stereo view.

Figure 3 is a computer image showing the backbone positions of the kinase loop A-loop 18 and helix αC 20 of BTK-KD (amino acids 397 to 659 of SEQ ID NO:2), phospho-LCK, and c-SRC, superimposed to illustrate their conformational differences and similarities.

Figure 4 is a computer image showing the non-inhibitory conformation of the A-loop 18 of BTK-KD (amino acids 397 to 659 of SEQ ID NO:2).

Figure 5 is a computer image showing the inhibitory conformation of the A-loop 18 of IRK.

Figure 6 is a model image of a proposed activation mechanism based on superimposed crystal structures of the kinase domains of BTK-KD (amino acids 397 to 659 of SEQ ID NO:2) and phospho-LCK. Helix αC 20 of BTK-KD (amino acids 397 to 659 of SEQ ID NO:2) is rotated 20° from the pivot point at residue L452 (SEQ ID NO:2). The unphosphorylated Y551 (SEQ ID NO:2) in the A-loop 10 of BTK-KD (amino acids 397 to 659 of SEQ ID NO:2) interacts with R544 (SEQ ID NO:2) via a hydroxyl group. The distance between the Cα position of residue D440 in BTK-KD (amino acids 397 to 659 of SEQ ID NO:2) and its counterpart in LCK is 6.7 Å.

Figure 7 is a diagrammatic representation of a proposed pathway for BTK (SEQ ID NO:2) catalysis activation, whereby R544 releases E445 to interact with

Y551 upon trans-phosphorylation, while E445 subsequently becomes bound to ATP. In contrast to previous predictions, the catalytic cleft of the BTK-KD (amino acids 397 to 659 of SEQ ID NO:2) is not occluded by the A-loop 18 or any other portion of the KD. Transphosphorylation of Y551 (SEQ ID NO:2) appears to trigger an exchange of hydrogen-bonded pairs from E445/R554 (SEQ ID NO:2) to E445/K430 (SEQ ID NO:2) causing subsequent relocation of helix αC 20 of the N-lobe (amino acids 397 to 475 of SEQ ID NO:2.

Figure 8 is a computer image of a backbone model of phosphorylated BTK-KD (amino acids 397 to 659 of SEQ ID NO:2) associated with ATP, Mg^{++} and the substrate Igα peptide. Mg^{++} ions (spheres), ATP triphosphate and Igα peptide substrate are shown in contact via hydrogen bond or electrostatic interaction (thin lines). The in-line phosphoryl transfer mechanism for BTK (SEQ ID NO:2) is proposed (indicated by arrows).

Figure 9 is a computer image of a space-filling model of phosphorylated BTK-KD (amino acids 397 to 659 of SEQ ID NO:2) associated with ATP, Mg^{++} and the substrate Igα peptide.

Figure 10 is a backbone model of the BTK kinase domain (amino acids 397 to 659 of SEQ ID NO:2), shown in stereo view, showing X-linked agammaglobulinaemia (XLA) related mutations of the BTK kinase domain (amino acids 397 to 659 of SEQ ID NO:2). As shown in Figure 10, XLA-associated BTK mutations involving the N-lobe 10 of the kinase domain (amino acids 397 to 475 of SEQ ID NO:2) are less frequent than those involving the C-lobe 20 (amino acids 479 to 659 of SEQ ID NO:2). A-loop 10 and helix αC 20 of BTK-KD (amino acids 397 to 659 of SEQ ID NO:2) are also shown.

Figure 11 shows an alignment of the amino acid sequence of human BTK kinase domain (amino acids 397 to 659 of SEQ ID NO:1) and murine BTK kinase domain (amino acids 397 to 659 of SEQ ID NO:2).

Brief Description of Sequences

SEQ ID NO:1 is an amino acid sequence of human BTK.

SEQ ID NO:2 is an amino acid sequence of murine BTK.

SEQ ID NO:3 is an amino acid sequence of the kinase domain of human BTK (I397-S659).

SEQ ID NO:4 is an amino acid sequence of the kinase domain of murine

BTK (I397-S659).

SEQ ID NO:5 is a nucleotide sequence of human BTK.

SEQ ID NO:6 is a nucleotide sequence of murine BTK.

SEQ ID NO:7 is an amino acid sequence of human BTK.

SEQ ID NO:8 is the amino acid sequence derived from data of Table 4 ~~5~~.

Abbreviations:

(Å) Ångström

(AA or aa) Amino acids

(AMP-PNP) 5'-Adenylylimidodiphosphate, Adenosine 5'[β,γ imido]triphosphate

(cAPK) cAMP-dependent kinase

(BCNU) 1,3-Bis(2-chloroethyl)-1-nitrosourea, or carmustine

(BLK) Tyrosine kinase, B-cell specific

(BMX) Tyrosine kinase, bone marrow, BTK/TEC family

(BTK) Bruton's tyrosine kinase, non-receptor tyrosine kinase

(CD28) T-cell surface antigen

(CD20) B1, B-lymphocyte surface antigen

(DISC) Death-inducing signaling complex; i.e. FAS, FADD, and FLICE (caspase-8)

(DMSO) Dimethyl sulfoxide

(DTT) Dithiothreitol

(EBV) Epstein Barr virus

(EDTA) Ethylene diamine tetraacetic acid

(EMP) Ethylene mercury phosphate

(EMT) ITK, Tyrosine kinase, expressed in T-cells and natural killer (NK) cells

(FADD) MORT1, FAS associating protein with death domain

(FAS) Transmembrane protein, intracellular death domain, mediates apoptosis

(FFT) Fast Fourier transform

(FGFRK) FGF receptor, tyrosine kinase domain

(FLICE) FADD-like ICE, Caspase-8, aspartate-specific cysteine protease

(HCK) Tyrosine kinase, hematopoetic cell-specific

(IDEC 8) Anti-CD20 monoclonal antibody

(IRK) Insulin receptor, tyrosine kinase domain

(KD) Kinase domain

(LCK) Tyrosine kinase, lymphocyte-specific

(LYN) Tyrosine kinase, T-cell expression

(NCS) Non-crystallographic symmetry

(NIDDM) Non-insulin-dependent diabetes mellitus

(PAGE) Polyacrylamide gel electrophoresis

(PEG) Polyethylene glycol

(PHK) Phosphorylase kinase

(PMSF) Phenylmethylsulfonyl fluoride

(PH) Pleckstrin homology

(PTK) Protein tyrosine kinase

(SDS) Sodium dodecyl sulfate

(SH1) SRC homology 1 domain, or kinase domain

(SH2) SRC homology 2 domain

(SH3) SRC homology 3 domain

(c-SRC) Tyrosine kinase homologous to v-SRC gene of Rous sarcoma virus

(SYK) Tyrosine kinase, spleen and thymus, widely expressed in hematopoetic cells

(TEC) Non-receptor tyrosine kinase, widely expressed in hematopoetic cells

(TXK) Tyrosine kinase, BTK/TEC family

(TRIS) 2-Amino-2-(hydroxymethyl)-1,3-propanediol

(XLA) X-linked agammaglobulinemia

Detailed Description of the Invention

Definitions:

The following definitions are used herein, unless otherwise described:

"Crystal" means the periodic arrangement of the unit cell (filled with the motif and its symmetry generated equivalents) into a lattice.

"Complementary or complement" as used herein, means the fit or relationship between two molecules that permits interaction, including for example, space, charge, three-dimensional configuration, and the like.

"Heavy atom derivative", as used herein, means a derivative produced by chemically modifying a crystal with a heavy atom such as Hg or Au.

"Kinase domain", as used herein, means the catalytic domain of BTK which has a consensus sequence in common with other protein tyrosine kinases, including TEC, BMX, BLK, EMT, and TXK. The catalytic activity of BTK refers to the

tyrosine phosphorylation of ligands such as the signal transduction protein, Igα. It is also termed the SH1 domain, in reference to the SRC homology domain 1.

"Ligand", as used herein, refers to an agent that associates with the BTK kinase domain, and may be an inhibitor or stimulator of BTK activity.

"Molecular complex", as used herein, refers to a combination of bound substrate or ligand with polypeptide, such as BTK with bound ATP, or BTK with bound Igα and ATP.

"Machine-readable data storage medium", as used herein, means a data storage material encoded with machine-readable data, wherein a machine programmed with instructions for using such data displays a graphical three-dimensional representation of molecules or molecular complexes.

"RD" kinase, as used herein, refers to protein kinases that have an arginine residue followed by an aspartic acid residue at the positions equivalent to the R520 and D521 residues in BTK. Examples include LCK (lymphocyte specific tyrosine kinase) and c-SRC.

"Scalable", as used herein, means the increasing or decreasing of distances between coordinates (configuration of points) by a scalar factor while keeping the angles essentially the same.

"Space group symmetry", as used herein, means the whole symmetry of the crystal that combines the translational symmetry of a crystalline lattice with the point group symmetry. A space group is designated by a capital letter identifying the lattice type (*P*, *A*, *F*, etc.) followed by the point group symbol in which the rotation and reflection elements are extended to include screw axes and glide planes. Note that the point group symmetry for a given space group can be determined by removing the cell centering symbol of the space group and replacing all screw axes by similar rotation axes and replacing all glide planes with mirror planes. The point group symmetry for a space group describes the true symmetry of its reciprocal lattice.

"Unit cell", as used herein, means the atoms in a crystal that are arranged in a regular repeating pattern, in which the smallest repeating unit is called the unit cell. The entire structure can be reconstructed from knowledge of the unit cell, which is characterized by three lengths (a, b and c) and three angles (α, β and γ). The quantities a and b are the lengths of the sides of the base of the cell and γ is the angle

between these two sides. The quantity c is the height of the unit cell. The angles α and β describe the angles between the base and the vertical sides of the unit cell.

"X-ray diffraction pattern" means the pattern obtained from X-ray scattering of the periodic assembly of molecules or atoms in a crystal. X-ray crystallography is an experimental technique that exploits the fact that X-rays are diffracted by crystals. It is not an imaging technique. X-rays have the proper wavelength (in the Ångström (Å) range, approximately 10^{-8} cm) to be scattered by the electron cloud of an atom of comparable size. Based on the diffraction pattern obtained from X-ray scattering of the periodic assembly of molecules or atoms in the crystal, the electron density can be reconstructed. Additional phase information must be extracted either from the diffraction data or from supplementing diffraction experiments to complete the reconstruction (the phase problem in crystallography). A model is then progressively built into the experimental electron density, refined against the data to produce an accurate molecular structure.

BTK/TEC Family of Proteins

The TEC family of non-receptor tyrosine kinases is composed of six proteins designated TEC, EMT (also designated ITK or TSK), BTK (previously designated ATK, BPK or EMB), BMX, TXK (also designated RLK) and Dsrc28C. All members of the family contain SH3 and SH2 domains and, with the exception of TXK and Dsrc28C, also contain pleckstrin homology (PH) and TEC homology (TH) domains in their amino termini. TEC shares the highest degree of amino acid homology with BTK (54%). Four alternatively spliced forms of TEC are expressed broadly in cells of hematopoietic lineage and hepatocytes. The 72 kDa EMT gene product associates with CD28 and becomes activated subsequent to CD28 ligation. The 80 kDa BMX protein seems to be expressed at highest levels in the heart. TXK expression is T-cell specific, while expression of the Drosophila TEC homolog, Dsrc28C, is developmentally regulated.

BTK

Bruton's tyrosine kinase (BTK) is a member of the SRC family of protein tyrosine kinases (PTKs), and in particular, the BTK/TEC family. It is a cytoplasmic PTK of 659 amino acids (aa) [SEQ ID NO:1, human]. The numbering of amino

acids for BTK, as used herein, represents the numbering of the human BTK sequence [SEQ ID NO:1].

The pleckstrin repeat homology (PH) domain (consensus, approximately 100 aa) is found in an N-terminal region at amino acid residues A2-R133 of SEQ ID NO: 1, followed by a BTK motif (consensus, approximately 36 aa) at amino acid residues N135-N170. The BTK motif is a zinc-binding motif containing conserved cysteines and a histidine, found C-terminal to the PH domain. The PH/Btk motif module has been called the TEC homology (TH) region. The SH3 domain (consensus, approximately 57 aa) spans the sequence of amino acid residues A221-I269 of SEQ ID NO: 1, while the SH2 homology domain (consensus, approximately 77 aa) spans the sequence of amino acid residues W281-V377 of SEQ ID NO: 1. SH3 (SRC homology 3) domains are often indicative of a protein involved in signal transduction related to cytoskeletal organization, which was first described in the SRC cytoplasmic tyrosine kinase. The structure is a partly opened beta barrel. The protein kinase homology domain (KD, approximately 256 aa) spans amino acid residues K400-E658 of SEQ ID NO: 1, while the ATP binding motif covers spans amino acid residues L408-V416 of SEQ ID NO: 1. The human BTK protein shares amino acid sequence identity with the SRC family of protein tyrosine kinases: TEC (54% amino acid conservation), BMX (48%), ITK (50%), and TXK (53%).

The BTK protein is approximately 98% conserved across its length (659 aa) between the human amino acid sequence [SEQ ID NO:1] and murine (M. musculus) amino acid sequence [SEQ ID NO:2], while it is approximately 99% conserved over the kinase domain. The amino acid changes across the kinase domain are conservative (K432R, K625R, T643S). The amino acid sequence of the BTK kinase domain is shown in ~~Table 1~~ Figure 11, comparing the published human [SEQ ID NO:3] and murine [SEQ ID NO:4] kinase domains.

Published BTK reference sequences include:

Human mRNA: H. sapiens GenBank (GB) access. no. NM_000061 [SEQ ID NO:5]

Murine mRNA: M. musculus, GB access. no. NM_013482 [SEQ ID NO:6]

Human protein: H. sapiens, GB access. no. XP_037089 [SEQ ID NO:7]

Human protein: H. sapiens, GB access. no. NP_000052 [SEQ ID NO:1]

Murine protein: M. musculus, GB access. no. NP_038510 [SEQ ID NO:2].

Table 1

BTK-Kinase Domain

436
IDPKDLTFLK ELGTGQFGVV KYGKWRGQYD VAIKMIKEGS
R
476
MSEDEFIEEA KVMMNLSHEK LVQLYGVCTK QRPIFIITEY
516
MANGCLLNYL REMRHRFQTQ QLLEMCKDVC EAMEYLESKQ
556
FLHRDLAARN CLVNDQGVVK VSDFGLSRYV LDDEYTSSVG
596
SKFPVRWSPP EVLMYSKFSS KSDIWAFGVL MWEIYSLGKM
636
PYERFTNSET AEHIAQGLRL YRPHLASEKV YTIMYSCWHE
R
659
KADERPTFKI LLSNILDVMD EES [hBTK-KD] SEQ ID NO :3
S [mBTK-KD] SEQ ID NO :4

Crystal Structure

The three-dimensional structure of BTK-KD was solved using X-ray crystallography to 2.1 Å resolution. Accordingly, the invention includes a BTK-KD crystal, as well as BTK-KD co-crystallized with a ligand, such as an inhibitor. The crystal has an orthorhombic space group symmetry, $P2_12_12_1$, and includes orthorhombic-shaped unit cells. Each unit cell has the approximate dimensions of: a=45 ± 5 Å, b=104 ± 10 Å, c=116 ± 10 Å, $\alpha=\beta=\gamma=90°$.

BTK-KD crystal structures according to the invention can be resolved using the methods described in the Examples below. BTK-KD can be crystallized in a non-complexed form or as a molecular complex with a ligand, for example an inhibitor that binds the kinase domain.

X-ray crystallographic analysis

Each of the constituent amino acids of BTK-KD is defined by a set of structure coordinates as set forth in Table 4 ~~5~~. The term "structure coordinates" refers to Cartesian coordinates derived from mathematical equations related to the patterns obtained on diffraction of a monochromatic beam of X-rays by the atoms (scattering centers) of a BTK-KD complex in crystal form. The diffraction data are used to calculate an electron density map of the repeating unit of the crystal. The electron density maps are then used to establish the positions of the individual atoms of the BTK-KD protein or protein/ligand complex.

Slight variations in structure coordinates can be generated by mathematically manipulating the BTK-KD or BTK-KD/ligand structure coordinates. For example, the structure coordinates as set forth in Table 4 ~~5~~ could be manipulated by crystallographic permutations of the structure coordinates, fractionalization of the structure coordinates, integer additions or subtractions to sets of the structure coordinates, inversion of the structure coordinates, or any combination of the above. Alternatively, modifications in the crystal structure due to mutations, additions, substitutions, and/or deletions of amino acids, or other changes in any of the components that make up the crystal, could also yield variations in structure coordinates. Such slight variations in the individual coordinates will have little effect on overall shape. If such variations are within an acceptable standard error as compared to the original coordinates, the resulting three-dimensional shape is considered to be structurally equivalent. Structural equivalence is described in more detail below.

It should be noted that slight variations in individual structure coordinates of the BTK-KD would not be expected to significantly alter the nature of chemical entities such as ligands that could associate with a kinase domain binding pocket. In this context, the phrase "associating with" refers to a condition of proximity between a ligand, or portions thereof, and a BTK molecule or portions thereof. The association may be non-covalent, wherein the juxtaposition is energetically favored by hydrogen bonding, van der Waals forces, or electrostatic interactions, or it may be covalent.

It will be readily apparent that the numbering of amino acids in other isoforms of BTK-KD may be different than that of the BTK-KD numbering disclosed herein.

Structural Features

Resolution of the BTK-KD (amino acids 397 to 659 of SEQ ID NO: 1) crystal structure revealed several structural features of the kinase domain as shown in Figure 1. The N-terminal lobe 10 (amino acid residues I397-E475 of SEQ ID NO: 1) contains five strands of anti-parallel β sheets (β1- β5) and one α-helix (αC). The C-terminal lobe 12 (amino acid residues N479-S659 of SEQ ID NO: 1) contains a 4-helix bundle flanked by a short antiparallel β sheet and four additional helices. The N- and C-lobes are connected by a linker region 14 (amino acid residues E475-N479 of SEQ ID NO: 1) and form a cleft 16 at the ATP binding site.

In contrast to previous predictions, the catalytic cleft of the BTK-KD is not occluded by the A-loop 18 or by any other portion of the KD. The A-loop 18 in the unphosphorylated BTK-KD structure adopts a unique non-inhibitory conformation very similar to the active state conformation of the A-loop in phosphorylated LCK-KD and hence does not limit substrate access to the active site (see Figure 3). Due to the inactive conformation of helix αC 20, however, the enzyme is not in the active state. Based on the BTK-KD structure here disclosed, transphosphorylation of Y551 (SEQ ID NO: 1) appears to trigger an exchange of hydrogen-bonded pairs from E445/R544 (SEQ ID NO: 1) to E445/K430 (SEQ ID NO: 1) causing subsequent relocation of helix αC 20 of the N-lobe 10, thereby inducing BTK activation (see Figure 7).

Modeling of the BTK Kinase Domain

Peptide substrate binding site

As shown in the examples, modeling of the crystal structure with a peptide substrate revealed a novel peptide substrate-binding site for BTK-KD.

The peptide substrate-binding site of BTK-KD is a shallow groove 16 Å long on the protein surface and can accommodate the binding of a portion of the target peptide substrate between the P-2 to P+3 positions. The first half of the binding site is a circular region of 5.8 Å in radius, centered around the P-1 carbonyl group. This region can bind the residues from P-2 to P, with the side chain groups of the P tyrosine and the P-1 residue being surrounded by the BTK-KD residues (Figures 8 and 9). The remaining atoms of the residues from P-2 to P are mostly exposed to the solvent environment.

An "enclosed" binding site is generally highly selective for peptide substrates whereas an "open" binding site is not. The cAPK crystal structure revealed an enclosed and negatively charged binding site for the Arg (P-1) residue (39). The PHK crystal structure demonstrated an enclosed polar binding site for Gln (P-2) formed by the P+1 loop which contains a Ser, Thr and Pro (32). In contrast, the BTK complex model suggests a half-buried and spacious P-1 binding site like the substrate binding site in IRK (18) (Figure 9). However, L483 of BTK (SEQ ID NO: 1) contributes to a preference for a hydrophobic P-1 residue whereas K1085 in IRK can be associated with a preference for a negatively charged P-1 residue.

SYK has an asparagine residue corresponding to L483 (SEQ ID NO: 1) and preferentially selects an aspartic acid residue for the P-1 residue over other types of residues (e. g. SYK selects a DYE motif (53)). Overall, the aliphatic portion of R525 (SEQ ID NO: 1) and the side chain groups of L483, C481, R487 and M596 (SEQ ID NO: 1) likely define the P-1 binding subsite. The sequence alignment of these residues with those of SRC family PTKs indicates a similar binding environment and therefore a similar recognition pattern for the P-1 position. c-SRC, BLK and LYN all preferentially select a leucine or isoleucine as the P-1 residue (54). Similarly, BTK is also likely to preferentially select a leucine or isoleucine as the P-1 residue, which is consistent with the notion that LY(223)D (SEQ ID NO: 1) is a more favored BTK autophosphorylation site than EY(551)TSS (52) (SEQ ID NO: 1).

The side chain group of the tyrosine targeted for phosphorylation on the substrate peptide is in contact with P560, R525, D521 (SEQ ID NO: 1), γ-phosphate and possibly with the side chain groups of Q412 (SEQ ID NO: 1) and K558 (SEQ ID NO: 1). The enclosed binding environment is consistent with a highly discriminating binding pocket for the P tyrosine.

The Glu (P+1) residue in BTK (SEQ ID NO: 1) is close to F559 of SEQ ID NO: 1 and interacts with N603 of SEQ ID NO: 1. Residues larger than Glu can potentially interact with residue S604 of SEQ ID NO: 1. Previous crystal structures for PTK kinase domains have not shown a specific and enclosed binding site for the P+1 residue, as well as in this current BTK-KD crystal structure. Therefore the selection for the P+1 residue is unlikely to be strict. However, in light of the differences for these three residues at the P+1 position, BTK is more similar to SRC

family PTKs than it is to IRK or SYK. Residues that correspond to F559, N603 and S604 of BTK (SEQ ID NO: 1) are specified in parentheses: IRK (L,N,E), SYK (K,G,S), SRC (F,N,R), LYN (F,N,A), BLK (F,N,P).

Our model is consistent with the phosphoryl transfer mechanism of an in-line nucleophilic attack. Specifically, D445 (SEQ ID NO: 1), K430 (SEQ ID NO: 1), a Mg ion, and α- and β-phosphate groups form a network of electrostatic interactions and hydrogen bonds presumably to align the ATP molecule in a conformation suitable for reaction (Figure 8). D539 (SEQ ID NO: 1) and the second Mg ion orient the γ-phosphate group for the in-line attack. The model indicates that the hydroxyl group of the P tyrosine forms a hydrogen bond with D521 (SEQ ID NO: 1), consistent with the acid residue.

TABLE ~~2~~ 1

Amino Acids in the BTK-KD Binding Pocket

Peptide binding loop (S557-P560 of SEQ ID NO: 1)

AA interacting with the P-1 residue (R525, L483, C481, R487, M596 of SEQ ID NO: 1)

AA interacting with the P residue (P560, R525, D521, Q412, K558 of SEQ ID NO: 1)

AA interacting with the P+1 residue (F559 and N603 of SEQ ID NO: 1)

AA interacting with Mg^{++} and ATP (D445, K430, and D539 of SEQ ID NO: 1)

Three-dimensional configurations

X-ray structure coordinates define a unique configuration of points in space. Those of skill in the art understand that a set of structure coordinates for a protein or a protein/ligand complex, or a portion thereof, define a relative set of points that, in turn, define a configuration in three dimensions. A similar or identical configuration can be defined by an entirely different set of coordinates, provided the distances and angles between coordinates remain essentially the same. In addition, a scalable configuration of points can be defined by increasing or decreasing the distances

between coordinates by a scalar factor, while keeping the angles essentially the same.

The present invention thus includes the scalable three-dimensional configuration of points derived from the structure coordinates of at least a portion of a BTK-kinase domain molecule or molecular complex, as well as structurally equivalent configurations, as described below. The scalable three-dimensional configuration includes points derived from structure coordinates representing the locations of a plurality of the amino acids defining the BTK-kinase domain ligand binding pocket, a BTK-KD substrate binding pocket, and the BTK-KD ATP binding site.

In one embodiment, the scalable three-dimensional configuration includes points derived from structure coordinates representing the locations of the backbone atoms of a plurality of amino acids defining the BTK-KD ligand binding pocket, a BTK-KD substrate binding pocket, and the BTK-KD ATP binding site. Alternatively, the scalable three-dimensional configuration includes points derived from structure coordinates representing the locations of the side chain and the backbone atoms (other than hydrogens) of a plurality of the amino acids defining the BTK-KD ligand binding pocket, a BTK-KD substrate binding pocket, and the BTK-KD ATP binding site, preferably the amino acids listed in Table 1 ~~2~~.

Specific amino acids defining a BTK-KD ligand binding pocket include those amino acids of the peptide binding loop (S557-P560 of SEQ ID NO: 1), those amino acids interacting with the P-1 residue (R525, L483, C481, R487, and M596 of SEQ ID NO: 1), those amino acids interacting with the P residue (P560, R525, D521, Q412, and K558 of SEQ ID NO: 1), those amino acids interacting with the P+1 residue (F559 and N603 of SEQ ID NO: 1), and those amino acids interacting with Mg^{++} and ATP (D445, K430, and D539 of SEQ ID NO: 1).

Likewise, the invention also includes the scalable three-dimensional configuration of points derived from structure coordinates of molecules or molecular complexes that are structurally homologous to BTK-KD, as well as structurally equivalent configurations. Structurally homologous molecules or molecular complexes are defined below. Advantageously, structurally homologous molecules can be identified using the structure coordinates of BTK-KD according to a method of the invention.

The configurations of points in space derived from structure coordinates according to the invention can be visualized as, for example, a holographic image, a stereodiagram, a model or a computer-displayed image, and the invention thus includes such images, diagrams or models.

Structurally equivalent crystal structures

Various computational analyses can be used to determine whether a molecule or a ligand binding pocket portion thereof is "structurally equivalent," defined in terms of its three-dimensional structure, to all or part of BTK-KD or its ligand binding pockets. Such analyses may be carried out in current software applications, such as the Molecular Similarity application of QUANTA (Molecular Simulations Inc., San Diego, CA), Version 4.1, and as described in the accompanying User's Guide.

The Molecular Similarity application permits comparisons between different structures, different conformations of the same structure, and different parts of the same structure. The procedure used in Molecular Similarity to compare structures is divided into four steps: (1) load the structures to be compared; (2) define the atom equivalences in these structures; (3) perform a fitting operation; and (4) analyze the results.

One structure is identified as the target (i.e., the fixed structure); all remaining structures are working structures (i.e., moving structures). Since atom equivalency within QUANTA is defined by user input, for the purpose of this invention equivalent atoms are defined as protein_backbone atoms (N, Cα, C, and O) for all conserved residues between the two structures being compared. A conserved residue is defined as a residue that is structurally or functionally equivalent. Only rigid fitting operations are considered.

When a rigid fitting method is used, the working structure is translated and rotated to obtain an optimum fit with the target structure. The fitting operation uses an algorithm that computes the optimum translation and rotation to be applied to the moving structure, such that the root mean square difference of the fit over the specified pairs of equivalent atom is an absolute minimum. This number, given in angstroms, is reported by QUANTA.

For the purpose of this invention, any molecule or molecular complex or ligand binding pocket thereof, or any portion thereof, that has a root mean square

deviation of conserved residue backbone atoms (N, Cα, C, O) of less than about 0.70 Å, when superimposed on the relevant backbone atoms is considered "structurally equivalent" to the reference molecule. That is to say, the crystal structures of those portions of the two molecules are substantially identical, within acceptable error. For example, structurally equivalent molecules or molecular complexes are those that are defined by the entire set of structure coordinates listed in Table 4 ~~5~~ ± a root mean square deviation from the conserved backbone atoms of those amino acids of not more than 0.70 Å.

The term "root mean square deviation" means the square root of the arithmetic mean of the squares of the deviations. It is a way to express the deviation or variation from a trend or object. For purposes of this invention, the "root mean square deviation" defines the variation in the backbone of a protein from the backbone of BTK-KD or a ligand binding pocket portion thereof, as defined by the structure coordinates of BTK-KD described herein.

Machine-readable storage media

Transformation of the structure coordinates for all or a portion of BTK-KD or the BTK-KD/ligand complex or one of its ligand binding pockets, for structurally homologous molecules as defined below, or for the structural equivalents of any of these molecules or molecular complexes as defined above, into three-dimensional graphical representations of the molecule or complex can be conveniently achieved through the use of commercially-available software.

The invention thus further provides a machine-readable storage medium including a data storage material encoded with machine-readable data wherein a machine programmed with instructions for using said data displays a graphical three-dimensional representation of any of the molecule or molecular complexes of this invention that have been described above. In a preferred embodiment, the machine-readable data storage medium includes a data storage material encoded with machine-readable data wherein a machine programmed with instructions for using said data displays a graphical three-dimensional representation of a molecule or molecular complex including all or any parts of a BTK-KD ligand binding pocket or a BTK-KD-like ligand binding pocket, as defined above. In another preferred embodiment, the machine-readable data storage medium includes a data storage material encoded with machine readable data wherein a machine programmed with

instructions for using said data displays a graphical three-dimensional representation of a molecule or molecular complex ± a root mean square deviation from the atoms of said amino acids of not more than 0.05 Å.

In an alternative embodiment, the machine-readable data storage medium includes a data storage material encoded with a first set of machine readable data which includes the Fourier transform of structure coordinates, and wherein a machine programmed with instructions for using said data is combined with a second set of machine readable data including the X-ray diffraction pattern of a molecule or molecular complex to determine at least a portion of the structure coordinates corresponding to the second set of machine readable data.

For example, a system for reading a data storage medium may include a computer including a central processing unit ("CPU"), a working memory which may be, e.g., RAM (random access memory) or "core" memory, mass storage memory (such as one or more disk drives or CD-ROM drives), one or more display devices (e.g., cathode-ray tube ("CRT") displays, light emitting diode ("LED") displays, liquid crystal displays ("LCDs"), electroluminescent displays, vacuum fluorescent displays, field emission displays ("FEDs"), plasma displays, projection panels, etc.), one or more user input devices (e.g., keyboards, microphones, mice, track balls, touch pads, etc.), one or more input lines, and one or more output lines, all of which are interconnected by a conventional bidirectional system bus. The system may be a stand-alone computer, or may be networked (e.g., through local area networks, wide area networks, intranets, extranets, or the internet) to other systems (e.g., computers, hosts, servers, etc.). The system may also include additional computer controlled devices such as consumer electronics and appliances.

Input hardware may be coupled to the computer by input lines and may be implemented in a variety of ways. Machine-readable data of this invention may be inputted via the use of a modem or modems connected by a telephone line or dedicated data line. Alternatively or additionally, the input hardware may include CD-ROM drives or disk drives. In conjunction with a display terminal, a keyboard may also be used as an input device.

Output hardware may be coupled to the computer by output lines and may similarly be implemented by conventional devices. By way of example, the output hardware may include a display device for displaying a graphical representation of a binding pocket of this invention using a program such as QUANTA as described

herein. Output hardware might also include a printer, so that hard copy output may be produced, or a disk drive, to store system output for later use.

In operation, a CPU coordinates the use of the various input and output devices, coordinates data accesses from mass storage devices, accesses to and from working memory, and determines the sequence of data processing steps. A number of programs may be used to process the machine-readable data of this invention. Such programs are discussed in reference to the computational methods of drug discovery as described herein. References to components of the hardware system are included as appropriate throughout the following description of the data storage medium.

Machine-readable storage devices useful in the present invention include, but are not limited to, magnetic devices, electrical devices, optical devices, and combinations thereof. Examples of such data storage devices include, but are not limited to, hard disk devices, CD devices, digital video disk devices, floppy disk devices, removable hard disk devices, magneto-optic disk devices, magnetic tape devices, flash memory devices, bubble memory devices, holographic storage devices, and any other mass storage peripheral device. It should be understood that these storage devices include necessary hardware (e.g., drives, controllers, power supplies, etc.) as well as any necessary media (e.g., disks, flash cards, etc.) to enable the storage of data.

Structurally homologous molecules, molecular complexes, and crystal structures

Structure coordinates can be used to aid in obtaining structural information about another crystallized molecule or molecular complex. The method of the invention allows determination of at least a portion of the three-dimensional structure of molecules or molecular complexes that contain one or more structural features that are similar to structural features of BTK-KD. These molecules are referred to herein as "structurally homologous" to BTK-KD. Similar structural features can include, for example, regions of amino acid identity, conserved active site or binding site motifs, and similarly arranged secondary structural elements (e.g., α helices and β sheets). Optionally, structural homology is determined by aligning the residues of the two amino acid sequences to optimize the number of identical amino acids along the lengths of their sequences; gaps in either or both sequences are permitted in making the alignment in order to optimize the number of

identical amino acids, although the amino acids in each sequence must nonetheless remain in their proper order. Two amino acid sequences are compared using the BLASTP program, version 2.0.9, of the BLAST 2 search algorithm, as described by Tatusova et al. (56), and available at the URL: ncbi.nlm.nih.gov/BLAST/. Preferably, the default values for all BLAST 2 search parameters are used, including matrix = BLOSUM62; open gap penalty = 11, extension gap penalty = 1, gap x_dropoff = 50, expect = 10, wordsize = 3, and filter on. In the comparison of two amino acid sequences using the BLAST search algorithm, structural similarity is referred to as "identity." Preferably, a structurally homologous molecule is a protein that has an amino acid sequence sharing at least 65% identity with a native or recombinant amino acid sequence of BTK-KD (for example, SEQ ID NO:3). More preferably, a protein that is structurally homologous to BTK-KD includes at least one contiguous stretch of at least 50 amino acids that shares at least 80% amino acid sequence identity with the analogous portion of the native or recombinant BTK-KD (for example, SEQ ID NO:3). Methods for generating structural information about the structurally homologous molecule or molecular complex are well known and include, for example, molecular replacement techniques.

Therefore, in another embodiment this invention provides a method of utilizing molecular replacement to obtain structural information about a molecule or molecular complex whose structure is unknown including the steps of:

(a) crystallizing the molecule or molecular complex of unknown structure;

(b) generating an X-ray diffraction pattern from said crystallized molecule or molecular complex; and

(c) applying at least a portion of the structure to the X-ray diffraction pattern to generate a three-dimensional electron density map of the molecule or molecular complex whose structure is unknown.

By using molecular replacement, all or part of the structure coordinates of BTK-KD or the BTK-KD/ligand complex as provided by this invention can be used to determine the unsolved structure of a crystallized molecule or molecular complex more quickly and efficiently than attempting to determine such information *ab initio.*

Molecular replacement can provide an accurate estimation of the phases for an unknown structure. Phases are one factor in equations that are used to solve crystal structures, and this factor cannot be determined directly. Obtaining accurate

values for the phases, by methods other than molecular replacement, can be a time-consuming process that involves iterative cycles of approximations and refinements and greatly hinders the solution of crystal structures. However, when the crystal structure of a protein containing at least a structurally homologous portion has been solved, the phases from the known structure provide a satisfactory estimate of the phases for the unknown structure.

Thus, this method involves generating a preliminary model of a molecule or molecular complex whose structure coordinates are unknown, by orienting and positioning the relevant portion of BTK-KD or the BTK-KD/ligand complex within the unit cell of the crystal of the unknown molecule or molecular complex. This orientation or positioning is conducted so as best to account for the observed X-ray diffraction pattern of the crystal of the molecule or molecular complex whose structure is unknown. Phases can then be calculated from this model and combined with the observed X-ray diffraction pattern amplitudes to generate an electron density map of the structure. This map, in turn, can be subjected to established and well-known model building and structure refinement techniques to provide a final, accurate structure of the unknown crystallized molecule or molecular complex (31).

Structural information about a portion of any crystallized molecule or molecular complex that is sufficiently structurally homologous to a portion of BTK-KD can be resolved by this method. In addition to a molecule that shares one or more structural features with BTK-KD as described above, a molecule that has similar bioactivity, such as the same catalytic activity, substrate specificity or ligand binding activity as BTK-KD, may also be sufficiently structurally homologous to BTK-KD to permit use of the structure coordinates of BTK-KD to solve its crystal structure.

In one embodiment of the invention, the method of molecular replacement is utilized to obtain structural information about a molecule or molecular complex, wherein the molecule or molecular complex includes at least one BTK-KD subunit or homolog. A "subunit" of BTK-KD is a BTK-KD molecule that has been truncated at the N-terminus or the C-terminus, or both. In the context of the present invention, a "homolog" of BTK-KD is a protein that contains one or more amino acid substitutions, deletions, additions, or rearrangements with respect to the amino acid sequence of BTK-KD (SEQ ID NO:3), but that, when folded into its native conformation, exhibits or is reasonably expected to exhibit at least a portion of the

tertiary (three-dimensional) structure of BTK-KD. For example, structurally homologous molecules can contain deletions or additions of one or more contiguous or noncontiguous amino acids, such as a loop or a domain. Structurally homologous molecules also include "modified" BTK-KD molecules that have been chemically or enzymatically derivatized at one or more constituent amino acid, including side chain modifications, backbone modifications, and N- and C- terminal modifications including acetylation, hydroxylation, methylation, amidation, and the attachment of carbohydrate or lipid moieties, cofactors, and the like.

A heavy atom derivative of BTK-KD is also included as a BTK-KD homolog. The term "heavy atom derivative" refers to derivatives of BTK-KD produced by chemically modifying a crystal of BTK-KD. In practice, a crystal is soaked in a solution containing heavy metal atom salts, or organometallic compounds, e.g., lead chloride, gold thiomalate, thiomersal or uranyl acetate, which can diffuse through the crystal and bind to the surface of the protein. The location(s) of the bound heavy metal atom(s) can be determined by X-ray diffraction analysis of the soaked crystal. This information, in turn, is used to generate the phase information used to construct three-dimensional structure of the protein (3).

The structure coordinates of BTK-KD as provided by this invention are particularly useful in solving the structure of BTK-KD mutants. Mutants may be prepared, for example, by expression of BTK-KD cDNA previously altered in its coding sequence by oligonucleotide-directed mutagenesis. Mutants may also be generated by site-specific incorporation of unnatural amino acids into BTK-KD proteins using the general biosynthetic method of Noren et al. (45). In this method, the codon encoding the amino acid of interest in wild-type BTK-KD is replaced by a "blank" nonsense codon, TAG, using oligonucleotide-directed mutagenesis. A suppressor tRNA directed against this codon is then chemically aminoacylated *in vitro* with the desired unnatural amino acid. The aminoacylated tRNA is then added to an *in vitro* translation system to yield a mutant BTK-KD with the site-specific incorporated unnatural amino acid.

The structure coordinates of BTK-KD are also particularly useful to solve or model the structure of crystals of BTK-KD, BTK-KD mutants, or BTK-KD homologs co-complexed with a variety of ligands. This approach enables the determination of the optimal sites for interaction between ligand entities, including candidate BTK-KD ligands and BTK-KD. Potential sites for modification within

the various binding sites of the molecule can also be identified. This information provides an additional tool for determining more efficient binding interactions, for example, increased hydrophobic interactions, between BTK-KD and a ligand. For example, high-resolution X-ray diffraction data collected from crystals exposed to different types of solvent allows the determination of where each type of solvent molecule resides. Small molecules that bind tightly to those sites can then be designed and synthesized and tested for their BTK inhibition activity.

All of the complexes referred to above may be studied using well-known X-ray diffraction techniques and may be refined versus 1.5-3.5 Å resolution X-ray data to an R-factor of about 0.30 or less using computer software, such as X-PLOR (Yale University, distributed by Molecular Simulations, Inc.; see, e.g., (3) and (37)). This information may thus be used to optimize known BTK modulators, and more importantly, to design new BTK modulators.

The invention also includes the unique three-dimensional configuration defined by a set of points defined by the structure coordinates for a molecule or molecular complex structurally homologous to BTK-KD as determined using the method of the present invention, structurally equivalent configurations, and magnetic storage media including such set of structure coordinates.

Further, the invention includes structurally homologous molecules as identified using the method of the invention.

Homology modeling

Using homology modeling, a computer model of a BTK-KD homolog can be built or refined without crystallizing the homolog. First, a preliminary model of the BTK-KD homolog is created by sequence alignment with BTK-KD, secondary structure prediction, the screening of structural libraries, or any combination of those techniques. Computational software may be used to carry out the sequence alignments and the secondary structure predictions. Structural incoherences, e.g., structural fragments around insertions and deletions, can be modeled by screening a structural library for peptides of the desired length and with a suitable conformation. For prediction of the side chain conformation, a side chain rotamer library may be employed. If the BTK-KD homolog has been crystallized, the final homology model can be used to solve the crystal structure of the homolog by molecular replacement, as described above. Next, the preliminary model is subjected to energy

minimization to yield an energy-minimized model. The energy-minimized model may contain regions where stereochemistry restraints are violated, in which case such regions are remodeled to obtain a final homology model. The homology model is positioned according to the results of molecular replacement, and subjected to further refinement including molecular dynamics calculations.

Specific Modulators of BTK That Interact with BTK-KD

Specific modulators of BTK include the inhibitor LFM-A13, a leflunomide metabolite, which docks within the ATP-binding pocket of the kinase domain (62). Using the IRK ternary structure as a template, a peptide hexamer derived from an ITAM motif of Igα (NLY*EGL), a known physiologic substrate of BTK, has been modeled into the peptide binding site of BTK-KD (33). See also U.S. Patent Nos. 6,294,575 (issued September 25, 2001) and 6,303,652 (issued October 16, 2001). Other inhibitors of BTK include calanolide derivatives (U.S. Patent No. 6,306,897, issued October 23, 2001) and coumarin derivatives (U.S. Patent No. 6,294,575, issued September 25, 2001).

Identification of Modulators of BTK

Potent and selective ligands that modulate BTK activity (inhibitors and stimulators) are identified using the three-dimensional homology model of the BTK kinase domain produced using the coordinates of Table 4 ~~5~~. Using this model, ligands that interact with the kinase domain are identified, and the result of the interactions is modeled. Agents identified as candidate molecules for modulating the activity of BTK are then screened against known bioassays. For example, the ability of an agent to inhibit the anti-apoptotic effects of BTK can be measured using assays known in the art, or for example, the assays disclosed in the Examples below. Using the modeling information and the assays described, one can identify agents that possess BTK-modulating properties.

Active Site and Other Structural Features

Applicants' invention provides information about the shape and structure of the substrate binding pocket of BTK-KD in the presence of a modulator.

Binding pockets are of significant utility in fields such as drug discovery. The association of natural ligands or substrates with the binding pockets of their corresponding receptors or enzymes is the basis of many biological mechanisms of

action. Similarly, many drugs exert their biological effects through association with the binding pockets of receptors and enzymes. Such associations may occur with all or any part of the binding pocket. An understanding of such associations helps lead to the design of drugs having more favorable associations with their target, and thus improved biological effects. Therefore, this information is valuable in designing potential modulators of BTK-KD ligand binding pockets, as discussed in more detail below.

The term "binding pocket," as used herein, refers to a region of a molecule or molecular complex that, as a result of its shape, favorably associates with a ligand. Thus, a binding pocket may include or consist of features such as cavities, surfaces, or interfaces between domains. Ligands that may associate with a binding pocket include, but are not limited to, cofactors, substrates, inhibitors, agonists, and antagonists.

The amino acid constituents of a BTK-KD ligand binding pocket as defined herein are positioned in three dimensions. In one aspect, the structure coordinates defining a ligand binding pocket of BTK-KD include structure coordinates of all atoms in the constituent amino acids; in another aspect, the structure coordinates of a ligand binding pocket include structure coordinates of just the backbone atoms of the constituent atoms.

The ligand binding pocket of BTK-KD for example, includes the amino acids listed in Table 1 ~~2~~. Alternatively, the ligand binding pocket of BTK may be defined by those amino acids whose backbone atoms are situated within about 5 Å of one or more constituent atoms of a bound substrate or ligand. In yet another alternative, the ligand binding pocket can be defined by those amino acids whose backbone atoms are situated within a sphere centered on the coordinates representing the alpha carbon atom of amino acid residue D521 of SEQ ID NO: 1, the sphere having a radius of about 5-6 Å, for example 5.8 Å.

The term "BTK-KD ligand binding pocket" includes all or a portion of a molecule or molecular complex whose shape is sufficiently similar to at least a portion of a ligand binding pocket of BTK-KD as to be expected to bind related structural analogues. A structurally equivalent ligand binding pocket is defined by a root mean square deviation from the structure coordinates of the backbone atoms of the amino acids that make up ligand binding pockets in BTK-KD of at most about 0.70 Å. This calculation is described below.

Accordingly, the invention provides molecules or molecular complexes including a BTK-KD ligand binding pocket or BTK-KD ligand binding pocket, as defined by the sets of structure coordinates described above.

Rational drug design

Computational techniques can be used to screen, identify, select and/or design ligands capable of associating with BTK-KD or structurally homologous molecules. Knowledge of the structure coordinates for BTK-KD permits the design and/or identification of synthetic compounds and/or other molecules that have a shape complementary to the conformation of the BTK-KD binding site. In particular, computational techniques can be used to identify or design ligands, such as inhibitors, agonists and antagonists, that associate with a BTK-KD ligand binding pocket or a BTK-KD ligand binding pocket. Inhibitors may bind to or interfere with all or a portion of an active site of BTK-KD, and can be competitive, non-competitive, or uncompetitive inhibitors. Once identified and screened for biological activity, these inhibitors, agonists, and/or antagonists may be used therapeutically or prophylactically, for example, to block BTK-KD activity and thus prevent the onset and/or further progression of diseases associated with BTK activity, such as XLA, and B-cell disorders, such as leukemia. Structure-activity data for analogues of ligands that bind to or interfere with BTK-KD ligand binding pockets can also be obtained computationally.

Data stored in a machine-readable storage medium that is capable of displaying a graphical three-dimensional representation of the structure of BTK-KD or a structurally homologous molecule, as identified herein, or portions thereof may thus be advantageously used for drug discovery. The structure coordinates of the ligand are used to generate a three-dimensional image that can be computationally fit to the three-dimensional image of BTK-KD or a structurally homologous molecule. The three-dimensional molecular structure encoded by the data in the data storage medium can then be computationally evaluated for its ability to associate with ligands. When the molecular structures encoded by the data is displayed in a graphical three-dimensional representation on a computer screen, the protein structure can also be visually inspected for potential association with ligands.

One embodiment of the method of drug design involves evaluating the potential association of a known ligand with BTK-KD or a structurally homologous

molecule, particularly with a BTK-KD ligand binding pocket. The method of drug design thus includes computationally evaluating the potential of a selected ligand to associate with any of the molecules or molecular complexes set forth above. This method includes the steps of: (a) employing computational means to perform a fitting operation between the selected ligand and a ligand binding pocket or a pocket nearby the ligand binding pocket of the molecule or molecular complex; and (b) analyzing the results of said fitting operation to quantify the association between the ligand and the ligand binding pocket.

In another embodiment, the method of drug design involves computer-assisted design of ligand that associate with BTK-KD, its homologs, or portions thereof. Ligands can be designed in a step-wise fashion, one fragment at a time, or may be designed as a whole or *de novo*.

To be a viable drug candidate, the ligand identified or designed according to the method must be capable of structurally associating with at least part of a BTK-KD ligand binding pocket, and must be able, sterically and energetically, to assume a conformation that allows it to associate with the BTK-KD ligand binding pocket. Non-covalent molecular interactions important in this association include hydrogen bonding, van der Waals interactions, hydrophobic interactions, and electrostatic interactions. Conformational considerations include the overall three-dimensional structure and orientation of the ligand in relation to the ligand binding pocket, and the spacing between various functional groups of a ligand that directly interact with the BTK-KD ligand binding pocket or homologs thereof.

Optionally, the potential binding of a ligand to a BTK-KD ligand binding pocket is analyzed using computer modeling techniques prior to the actual synthesis and testing of the ligand. If these computational experiments suggest insufficient interaction and association between it and the BTK-KD ligand binding pocket, testing of the ligand is obviated. However, if computer modeling indicates a strong interaction, the molecule may then be synthesized and tested for its ability to bind to or interfere with a BTK-KD ligand binding pocket. Binding assays to determine if a compound actually modulates with BTK activity can also be performed and are well known in the art.

Several methods can be used to screen ligands or fragments for the ability to associate with a BTK-KD ligand binding pocket. This process may begin by visual inspection of, for example, a BTK-KD ligand binding pocket on the computer screen

based on the BTK-KD structure coordinates or other coordinates which define a similar shape generated from the machine-readable storage medium. Selected ligands may then be positioned in a variety of orientations, or docked, within the ligand binding pocket. Docking may be accomplished using software such as QUANTA and SYBYL, followed by energy minimization and molecular dynamics with standard molecular mechanics forcefields, such as CHARMM and AMBER.

Specialized computer programs may also assist in the process of selecting ligands. Examples include GRID (17); MCSS (38) available from Molecular Simulations, San Diego, CA); AUTODOCK (13) available from Scripps Research Institute, La Jolla, CA); and DOCK (29) available from University of California, San Francisco, CA).

BTK-KD binding ligands can be designed to fit a BTK-KD binding site, optionally as defined by the binding of a known modulator. There are many ligand design methods including, without limitation, LUDI (4); available from Molecular Simulations Inc., San Diego, CA); LEGEND (42); available from Molecular Simulations Inc., San Diego, CA); LeapFrog (available from Tripos Associates, St. Louis, MO); and SPROUT (10); available from the University of Leeds, UK).

Once a compound has been designed or selected by the above methods, the efficiency with which that ligand may bind to or interfere with a BTK-KD ligand binding pocket may be tested and optimized by computational evaluation. For example, an effective BTK-KD ligand binding pocket ligand should preferably demonstrate a relatively small difference in energy between its bound and free states (i.e., a small deformation energy of binding). Thus, an efficient BTK-KD ligand binding pocket ligands should preferably be designed with a deformation energy of binding of not greater than about 10 kcal/mole; more preferably, not greater than 7 kcal/mole. BTK-KD ligand binding pocket ligands may interact with the ligand binding pocket in more than one conformation that is similar in overall binding energy. In those cases, the deformation energy of binding is taken to be the difference between the free energy of the ligand and the average energy of the conformations observed when the ligand binds to the protein.

A ligand designed or selected as binding to or interfering with a BTK-KD ligand binding pocket may be further computationally optimized so that in its bound state it would preferably lack repulsive electrostatic interaction with the target enzyme and with the surrounding water molecules. Such non-complementary

electrostatic interactions include repulsive charge-charge, dipole-dipole, and charge-dipole interactions.

Specific computer software is available to evaluate compound deformation energy and electrostatic interactions. Examples of programs designed for such uses include: Gaussian 94, revision C (M.J. Frisch, Gaussian, Inc., Pittsburgh, PA); AMBER, version 4.1 (P.A. Kollman, University of California at San Francisco,); QUANTA/CHARMM (Molecular Simulations, Inc., San Diego, CA); Insight II/Discover (Molecular Simulations, Inc., San Diego, CA); DelPhi (Molecular Simulations, Inc., San Diego, CA); and AMSOL (Quantum Chemistry Program Exchange, Indiana University). These programs can be implemented, for instance, using a Silicon Graphics workstation, such as an Indigo2 with IMPACT graphics. Other hardware systems and software packages will be known to those skilled in the art.

Another approach encompassed by this invention is the computational screening of small molecule databases for ligands or compounds that can bind in whole, or in part, to a BTK-KD ligand binding pocket. In this screening, the quality of fit of such ligands to the binding site may be judged either by shape complementarity or by estimated interaction energy (35).

A compound that is identified or designed as a result of any of these methods can be obtained (or synthesized) and tested for its biological activity, e.g., inhibition of BTK activity.

Therapeutic Use

B-cells and B-cell precursors expressing BTK have been implicated in the pathology of a number of diseases and conditions including B-cell malignancies (e.g., acute lymphoblastic leukemia, chronic lymphocytic leukemia, non-Hodgkin's lymphoma, EBV lymphomia, and myeloma), other cancers, B-cell lymphoproliferative disorders/autoimmune diseases (e.g., lupus, Crohn's disease, and chronic or graft-versus-host disease), mast cell disorders (e.g., allergies, and anaphylactic shock), conditions that relate to improper platelet aggregation, and rejection of xenotransplants (e.g., pig to human heart transplants).

BTK inhibitors designed or identified using the crystal structure of the BTK-KD can be used to treat disorders where inhibition or prevention of a TEC family kinase is indicated. For cancer cells expressing BTK, e.g. leukemia and lymphoma

cells, BTK inhibitors may kill or chemosensitize. In autoimmune disease such as Lupus or autoimmune diabetes, BTK inhibitors may halt antibody production. In graft-versus-host disease after bone marrow transplantation, these inhibitors may abrogate the B-lymphocyte mediated component of the graft rejection. Similarly designed inhibitors may be useful in organ transplantation, especially in patients with chronic rejection of organs such as liver, pancreas, and kidney. And in xenotransplantation, in which rejection is mediated by B-cells, these inhibitors may also be useful. BTK inhibitors may prevent the formation of blood clots in thrombophilia (a tendency to develop blot clots). In allergy, anaphlaxis, and asthma, the goal would be to inhibit the mast cell response.

BTK inhibitors are also useful as chemosensitizing agents, useful in combination with other chemotherapeutic drugs, in particular, drugs that induce apoptosis. Examples of other chemotherapeutic drugs that can be used in combination with chemosensitizing BTK inhibitors include topoisomerase I inhibitors (e.g., camptothesin or topotecan), topoisomerase II inhibitors (e.g., daunomycin and etoposide), alkylating agents (e.g., cyclophosphamide, melphalan and BCNU), tubulin-directed agents (e.g., taxol and vinblastine), and biological agents (e.g., antibodies such as anti CD20 antibody, IDEC 8, immunotoxins, and cytokines).

BTK stimulators designed or identified using the crystal structure of the BTK-KD can be used to treat disorders, where induction of BTK activity is indicated, for example, in the treatment of B-cell disorders or immunodeficiencies, such as XLA, and in particular to stimulate differentiation of B-cells. In patients with infectious diseases, the goal would be to enhance natural B-cell mediated immunity during the course of infection. In cancer patients, BTK stimulators may boost the immune system by increasing the ability of B-cells to produce antibodies and thus the state of alertness of the B-cell (humoral) compartment of the immune system. By boosting the B-cell immune response through stimulation of BTK, the success of vaccination may be enhanced.

The invention is illustrated by the following non-limiting Examples.

EXAMPLES

Example 1: Subcloning and Expression of the Murine BTK Kinase Domain

Subcloning

The murine BTK kinase domain (BTK-KD, residues I397 to S659 of amino acids 397 to 659 of SEQ ID NO: 2) was amplified from the wild-type BTK gene (GB access. no. NM_013482 SEQ ID NO: 6) by PCR. The PCR product was cloned into the pCR2.1 vector (BTK-KD/pCR2.1) using the Invitrogen TA cloning procedure (Invitrogen LTI, Carlsbad, CA). Subsequently, the BTK-KD/pCR2.1 was completely digested with *Nco*I and *Hind*III. The fragment was purified and ligated to the pFastBac HTb donor plasmid (Invitrogen LTI), generating pFastBac HTb/BTK-KD. The vector construct was then used to produce a baculoviral stock using the Bac-to-Bac baculovirus expression system (Invitrogen LTI). The expression was checked by the anti-BTK antibody, C-20 (Santa Cruz Biotechnology, Santa Cruz, CA) and by anti-6-Histidine antibody.

Expression

Spodoptera frugiperda (Sf9) cells were maintained at 27°C in Sf-900 II SFM (GibcoBRL) containing 50 units/ml penicillin and 50 µg/ml streptomycin. Cells at a density of 1 - 1.5 X 10^6 cells/ml were infected with the recombinant BTK-KD- (of amino acids 397 to 659 of SEQ ID NO: 2) containing virus at a 5-fold multiplicity of infection. After 54 hours post-infection, the cells were harvested by centrifugation at 800 g for 10 minutes, washed with phosphate-buffered saline, then flash-frozen in a dry ice/ethanol bath and finally stored at -80°C.

Purification

The frozen cells were thawed in a 37°C water bath, resuspended in 5 volumes of lysis buffer (50 mM TRIS/HCl pH=8.5, 100 mM KCl, 2mM DTT and 1mM PMSF), and then sonicated for 1 minute and centrifuged at 30,000g for 45 minutes. The supernatant was loaded onto a Ni^{2+} column, equilibrated with a solution containing 10 mM TRIS/HCl buffer, pH = 8.0, 500 mM KCl and 0.5 mM DTT at a flow rate of 0.75 ml/min. The column was washed with 20-bed volumes of buffer A (20 mM TRIS/HCl, pH = 8.5, 500 mM KCl, 15-20 mM imidazole and 2 mM DTT), and then washed with 10-bed volumes of buffer B (20 mM TRIS/HCl,

pH = 8.5, 1 M KCl and 2 mM DTT). Afterwards, it was washed again with 2-bed volumes of buffer A. The protein was eluted with buffer C (20 mM TRIS/HCl, 100 mM KCl, 150 mM imidazole and 2 mM DTT).

Fractions that contained BTK-KD (amino acids 397 to 659 of SEQ ID NO: 2) were pooled and dialyzed against a solution containing 20 mM TRIS/HCl, 100 mM NaCl, 2 mM DTT and 1 mM EDTA. The protein was concentrated to 5 mg/ml, digested with rTEV protease (6 μg/mg) at 4°C overnight to remove the poly-His tag, and concentrated to 3 ml. Concentrated protein was then loaded onto a SUPRADEX 200 column (26 x 60 cm, Amersham Pharmacia Biotech AB, Uppsala, Sweden), equilibrated with a solution of 20 mM TRIS/HCl, pH=8.5, 50 mM NaCl and 2 mM DTT. The purified BTK-KD (amino acids 397 to 659 of SEQ ID NO: 2) fraction was concentrated to 12 mg/ml for crystallization.

The purity of the BTK-KD (amino acids 397 to 659 of SEQ ID NO: 2) polypeptide was confirmed by PAGE analysis with Coomassie blue staining, and by Western blot analysis probed with an anti-BTK antibody. Western blot analysis probed with an anti-phosphotyrosine antibody indicated that the purified BTK-KD (amino acids 397 to 659 of SEQ ID NO: 2) was not phosphorylated. *In vitro* kinase assays indicated that the nonphosphorylated BTK-KD (amino acids 397 to 659 of SEQ ID NO: 2) was able to be phosphorylated and to transfer the phosphate group to a GST fusion protein of Igα in a 5 minute kinase reaction.

Materials and Methods: Immunoprecipitation and Kinase Assays of Recombinant Proteins from Insect Cells

Immunoprecipitations, immune-complex protein kinase assays, and immunoblotting using the ECL chemiluminescence detection system (Amersham Life Sciences, Oakbrook, IL) were conducted as described previously (33, 64, 12, 60). Following electrophoresis, kinase gels were dried onto WHATMAN 3M filter paper and subjected to phosphoimaging on a Molecular Imager (Bio-Rad, Hercules, CA) as well as autoradiography on film. Similarly, all chemiluminescent BTK Western blots were subjected to three dimensional densitometric scanning using the Molecular Imager and Imaging Densitometer with MOLECULAR ANALYST/MACINTOSH version 2.1 software following the specifications of the manufacturer (Bio-Rad). For each compound concentration, a BTK kinase activity index was determined by comparing the ratios of the kinase activity in

phosphorimager units (PIU) and density of the protein bands in densitometric scanning units (DSU) to those of the baseline sample and using the formula: Activity Index = [PIU of kinase band/DSU of BTK protein band]$_{\text{test sample}}$: [PIU of kinase band/DSU of BTK protein band]$_{\text{baseline control sample}}$. GST-Igα was sometimes used as an exogenous substrate for BTK immune-complex protein kinase assays, as described (33). Horseradish peroxidase-conjugated sheep anti-mouse, donkey anti-rabbit secondary antibodies and ECL reagents were purchased from Amersham.

Sf21 cells were infected with a baculovirus expression vector for full-length BTK (SEQ ID NO: 2), as described briefly below. Cells were harvested, lysed (10mM TRIS pH7.6, 100mM NaCl, 1% NONIDET P-40, 10% glycerol, 50mM NaF, 100mM Na_3VO_4, 50 μg/ml phenylmethylsulfonyl fluoride (PMSF), 10 μg/ml aprotonin, μg/ml leupeptin), and the kinases were immunoprecipitated from the lysates, as reported (64). The antibody used for immunoprecipitation of BTK (SEQ ID NO: 2) from insect cells was polyclonal rabbit anti-BTK serum (33). Kinase assays were performed following a 1 hour exposure of the immunoprecipitated tyrosine kinases to the test compounds, as described below (33, 60). The immunoprecipitates were subjected to Western blot analysis as previously described (64).

Example 2: Crystallization of the BTK Kinase Domain of SEQ ID NO: 4 (corresponding to amino acid residues 397 to 659 of SEQ ID NO: 2)

The pure protein at a concentration of 2 mg/ml was used for dynamic light scattering studies. The data indicated the BTK-KD (amino acids 397 to 659 of SEQ ID NO: 2) sample was mono-disperse immediately after purification, but became poly-disperse within 30 minutes at room temperature. Therefore, all crystallization was performed at 4°C.

Crystallization

The purified BTK-KD (amino acids 397 to 659 of SEQ ID NO: 2) was crystallized at 4°C using the hanging drop method, with 2 μl of protein and 1 μl of reservoir solution in the drop and equilibrated with 600 μl of reservoir solution containing 20 % PEG-1000, 100 mM TRIS/HCl, pH = 8.0 and 1 mM DTT using VDP trays (Hampton Research, Laguna Niguel, CA). The crystals began to appear within one week, which reached a full size of 200 x 200 x 200 μm in 2 to 3 weeks.

Example 3: Structural Analysis of the BTK Kinase Domain Crystal

Data collection

Crystals were analyzed using a CCD detector and high-intensity synchrotron radiation source at the Cornell High Energy Synchrotron Source (CHESS, F2 Station, Cornell University, Ithaca, NY). Data collected include two native data sets (Nat 1 and Nat 2) and two heavy-atom derivative data sets (EMP and AU). Data statistics are summarized in Table 2 ~~3~~. One crystal was soaked for 24 hours in 5 mM $K_2Au(CN)_2$ or (AU), and another crystal was soaked in 0.1 mM ethylene mercury phosphate (EMP). All crystals were flash-cooled and kept in liquid nitrogen with 30% PEG-1000 solution as a natural cryoprotectant. All data sets were processed using DENZO and SCALEPACK programs (40), and analyzed and scaled using the CCP4 program suite (7). The data showed that the BTK-KD (amino acids 397 to 659 of SEQ ID NO: 2) crystal belongs to the $P2_12_12_1$ space group with cell dimensions $a = 45$ Å, $b = 104$ Å and $c = 116$ Å.

Molecular replacement

The native data set was analyzed for molecular replacement solution using AMoRe (7, 40). The self-rotation function calculation failed to indicate any non-crystallographic symmetry (NCS), suggesting that there is either no NCS or that the NCS axis is too close to the crystallographic axis (in fact, the 2-fold axis was later found to be close to the X axis).

The search models of polyglycine and polyalanine from crystal structures of kinase domains, including LCK, IRK, FGFRK, HCK and SRC as well as the homology BTK kinase domain model (U.S. Patent No. 6,294,575, issued September 25, 2001), revealed a clear solution in rotation function searches with a top peak 10 - 25 % higher than the second solution, depending on the search model used in the calculation. The search model of LCK with the activation loop yielded better results, but the apo-IRK model with the activation loop produced noisy results. This correlates with the refined BTK structure defined herein, where the activation loop of the BTK-KD (amino acids 397 to 659 of SEQ ID NO: 2) is similar to that of phospho-LCK, but not IRK. Translational searches using both the polyglycine/polyalanine models and the models which maintain conserved residues failed to produce a convincing solution, likely due to the existence of two molecules

in the asymmetric unit and the significant difference between the search models and the target structure.

Multiple isomorphous replacement

A heavy atom derivative search using a Patterson function calculation (in the RSPS program) followed by difference Fourier calculation (FFT) in the CCP4 suite (7) based on the heavy atom derivative data sets identified four Hg sites and six Au sites. These sites were used to phase all reflections at 4.0 Å and above by MLPHARE ((7), CCP4 suite). The correct handedness of the protein was determined by the sign of anomalous occupancies during the heavy atom site refinement. The map calculated from the combination of Hg and Au derivative phase information, including anomalous diffraction data of Hg atoms in the EMP derivative, was subject to several rounds of phase improvement using the DM program ((7), CCP4 suite) with a solvent flattening and histogram matching method. The improved maps demonstrated clear boundaries between the target protein and solvent region. The maps indicated two BTK-KD (amino acids 397 to 659 of SEQ ID NO: 2) molecules in one asymmetric unit. Therefore, two polyglycine/polyalanine kinase search models were manually fit into the electron density and revealed how the two molecules are related by NCS. The matrix that relates the orientation of the two molecules was generated and refined into two different matrices corresponding to the N-lobe and C-lobe domains, respectively, using MAMA and 6D_IMP (26). The refined matrices were used in multi-domain averaging of the electron density map using 6D_AVE (26). The final map was considerably improved from the previous map with α-helix and β-strand structures, as well as many large amino acids clearly visible. The approximately five hundred amino acid residues (2 x 263 aa) and approximately 4000 atoms of the two BTK-KD (amino acids 397 to 659 of SEQ ID NO: 2) molecules based on the BTK amino acid sequence (SEQ ID NO: 2) were readily fit into the electron density map. The entire amino acid sequence of the BTK fragment starting from amino acid residue I397 to residue S659 of SEQ ID NO: 2 were mostly traceable in the electron density map, except for a few disordered amino acid residues on the molecular surface (see Figure 2).

Crystallographic refinement

The kinase domain structures of the two BTK molecules (amino acids 397 to 659 of SEQ ID NO: 2) were refined using simulated annealing in X-PLOR (6) and numerous structural adjustments were performed with help of CHAIN (53) and O programs (24). The refinement statistics are summarized in Table 2 ~~3~~.

The final structure was refined at 2.1 Å resolution to an R-factor of 22% with all amino acid residues falling into favored or generously allowed regions in the Ramachandran plot (except for glycine residues), as indicated by PROCHECK (13). The average B-factor for all nonhydrogen atoms is 21 $Å^2$ and is below 20 $Å^2$ for more than half of the protein atoms. Two short regions that are disordered in the electron density map include part of the β1 strand (residues G409-Q412 of SEQ ID NO: 2) and part of the activation (A)-loop (residues E550 and V555 of SEQ ID NO: 2). Other regions that display a visible electron density in the original map and have high B-factors include the loop from residues V546 to D549 of SEQ ID NO: 2, the loops around residue Q467 of SEQ ID NO: 2, and the N-terminal end of helix αC that has B-factors mostly in the 20-30 $Å^2$ range.

Overall architecture of the BTK kinase domain

A computer graphic of the BTK-KD (amino acids 397 to 659 of SEQ ID NO: 2) crystal structure in its unphosphorylated state is shown in Figure 1 as a ribbon representation. BTK-KD (amino acids 397 to 659 of SEQ ID NO: 2) is packed in a dimeric form in the crystal lattice, but present mainly in monomeric form in solution (data not shown). The N-lobe and C-lobe of both BTK kinase molecules (amino acids 397 to 659 of SEQ ID NO: 2) is shown. The secondary structure is labeled only on one molecule. The two BTK kinase domain molecules (amino acids 397 to 659 of SEQ ID NO: 2) are related by a non-crystallographic two-fold axis that is approximately vertical in the center. This figure was prepared using MOLSCRIPT (28) and RASTER3D programs (36).

BTK-KD (amino acids 397 to 659 of SEQ ID NO: 2) has a two-lobe fold reminiscent of the topology of other PTK kinase domain structures (14, 15). The secondary structure of the BTK-KD (amino acids 397 to 659 of SEQ ID NO: 2) is labeled in Figure 1 using the established nomenclature (27, 71). The N-terminal lobe (residues I397-E475 of SEQ ID NO: 2) contains five strands of anti-parallel β sheets (β1-β5) and one α-helix (helix αC) (shown in Figure 1). The C-terminal lobe

(residues N479-S659 of SEQ ID NO: 2) contains a 4-helix bundle (αD, αE, αF and αH) flanked by a short antiparallel β sheet (β6, β8 and β9) and four additional helices (αI, αDE, αEF, and αHI). The two helical structural segments that are too short to be labeled in the Figures, i.e. αDE and αHI, are located between alpha helices D and E and between H and I, respectively. The N- and C-lobes are connected by a linker region (residues E475-N479 of SEQ ID NO: 2) and form a cleft at the ATP binding site.

TABLE 2 3

Statistics for Crystallographic Data Analysis of the BTK Kinase Domain[#]

Crystal	Nat 1	Nat 2	EMP	Au
X-ray source, wavelength (Å)	CHESS, λ=1.009	CHESS, λ=1.009	CHESS, λ=1.009	CHESS, λ=1.009
Resolution limits (Å)	2.1	3.0	3.0	3.0
Unique reflections	25,284	10,020	11,391	10,028
Completeness (%)	80.4 (79)*	86.7(81)	96.5 (79)	88.3 (68)
Rsym (%)	5.4 (20)	8.7 (21)	8.0 (19)	8.7 (23)
MIRAS analysis				
Resolution range (Å)			15-4	15-4
Sites			4	6
Cullis R-factor (%)			66	82
Phasing Power			1.21	0.73
Overall FOM			0.6	
Refinement				
Resolution range (Å)	5 - 2.1			
Reflections used (F> 2σ)	20370			
Total nonhydrogen atoms (protein)	4180			
Water molecules	180			
R_{cryst} (%)	22.1			
R_{free} (%)	28.7			
Rmsd from ideal bond length	0.006			
Rmsd from ideal bond angle	1.5			
Average B (Å^2)	19.8			
(for 95% of protein atoms with a B factor < 40.0 Å^2)				

Data for the outermost resolution shell are given in parentheses.

$R_{sym} = \sum_h \sum_{i=1}^{N} \left| \bar{I}(h) - I_i(h) \right| / \sum_h \sum_{i=1}^{N} I_i(h) * 100$, where $I_i(h)$ is the ith measurement of reflection h and $\bar{I}(h)$ is the mean value of the N equivalent reflections.

$R_{cullis} = \sum \left| F_{PH} \pm F_P \right| - F_{H(calc)} \left| / \sum \right| F_{PH} + F_P \right|$ for all centric reflections.

Phasing power = rms($|F_H|$/E), where $|F_H|$ is the heavy atom structure factor amplitude and E is the residual lack of closure.

$R_{cryst} = \Sigma ||F_{obs}| - |F_{calc}|| / \Sigma |F_{obs}|$, where summation is over data used in the refinement.

R_{free} is the same as R_{cryst} but only include 5% of data excluded from refinement.

* Reflections were not used in the resolution bins near or on *ice* rings.

[#] Amino acids 397 to 659 of SEQ ID NO: 2

Example 7: Structural Comparison

The BTK-KD (amino acids 397 to 659 of SEQ ID NO: 2) crystal structure was compared with the crystal structures of other kinase domains including those of c-APK (PDB access code: 1ATP), LCK (3LCK), c-SRC (2SRC), HCK (1QCF), FGFRK (1AGW), IRK (1IRK for the apo structure; and 1IR3 for the ternary complex) using CHAIN and O (24, 53).

c-AMP-Dependent Protein Kinase (E.C.2.7.1.37) (cAPK) (Catalytic Subunit) Complex With The Peptide Inhibitor PKI (5-24) And MnATP (A Ternary Complex Of cAPK)

Phosphorylated Insulin Receptor Tyrosine Kinase In Complex With Peptide Substrate And Atp Analog

Figure 3 shows the backbone positions of the A-loop and helix αC for BTK-KD (amino acids 397 to 659 of SEQ ID NO: 2), phospho-LCK, and c-SRC, superimposed to illustrate their conformational differences and similarities. An AMP-PNP molecule is present in the c-SRC crystal structure and was used to mark the location of active site. The side chains of R544 and Y551 in BTK (SEQ ID NO: 1) and their equivalent residues in LCK and c-SRC on the A-loop are shown. All coordinates were superimposed in CHAIN (53). This figure was prepared using the INSIGHT II program suite (1997, Molecular Simulations, Inc., San Diego, CA).

BTK-KD (amino acids 397 to 659 of SEQ ID NO: 2) has a two-lobe fold with some similarity to that of other kinase domains and some differences. The rotation of the N-lobe relative to the C-lobe varies among the different KD structures and the ATP-binding cleft between the two lobes is closed when substrates or analogs are bound (18, 39). Therefore, both lobes of a KD need to adopt a mandatory closed conformation for the kinase domain to achieve a catalytically active state. The crystal structure of the unphosphorylated BTK kinase domain (amino acids 397 to 659 of SEQ ID NO: 2) revealed that its N- and C-terminal lobes adopt a closed conformation very similar to the reported conformation of the lobes of the phosphorylated LCK- KD (root-mean-square deviation between the backbones of the central portion of β3 and β5 < 1 Å (71), and the central regions of the β3 and β5 strands are almost superimposable when the C-lobes are overlaid. See Figure 3. However, the β1 and β2 strands, very much like the corresponding β

strands of the cAPK-KD, adopt a more "closed" conformation than their counterparts in LCK-KD. The rotation needed to superimpose the N-lobe of the BTK-KD (amino acids 397 to 659 of SEQ ID NO: 2) onto the N-lobe the cAPK-KD is only 5.2°, whereas an 11° rotation is required to overlay the N-lobe of the LCK-KD with the N-lobe of the cAPK-KD (39). By comparison, the magnitudes of the rotation needed to open the BTK-KD (amino acids 397 to 659 of SEQ ID NO: 2) and LCK-KD N-lobes to match the conformation observed in the apo-IRK structure are 22° and 17° (39), respectively.

In contrast to the similarity of the closed conformation of their N- and C-terminal lobes, the C-terminal ends of the helix αC in unphosphorylated BTK-KD (amino acids 397 to 659 of SEQ ID NO: 2) versus phosphorylated LCK-KD are markedly different (see Figure 3) where black lines indicate hydrogen bonds. The distance between the Cα position of residue D440 in BTK-KD (amino acids 397 to 659 of SEQ ID NO: 2) and its counterpart in LCK is 6.7 Å. From the pivot point at residue F452, helix αC of BTK-KD (amino acids 397 to 659 of SEQ ID NO: 2) needs to be rotated towards the ATP-binding cleft by 20° to be superimposed onto the helix αC of the LCK-KD. The helix αC in phosphorylated LCK-KD adopts a closed conformation consistent with a catalytically active state (71). By comparison, the helix αC of the unphosphorylated BTK-KD (amino acids 397 to 659 of SEQ ID NO: 2) adopts a more open conformation than that of the LCK-KD. The conformation of helix αC of the BTK-KD (amino acids 397 to 659 of SEQ ID NO: 2) is different from the open conformation of helix αC in c-SRC as well (see Figure 3), in accordance with a unique conformation of the A-loop in BTK-KD (amino acids 397 to 659 of SEQ ID NO: 2). Significant structural differences between BTK-KD (amino acids 397 to 659 of SEQ ID NO: 2) and LCK-KD were also found in helices αDE, αEF, αG and αI (which differed in location by approximately 2 Å), and in the glycine loop (β1↑β2). The β1 strand of the glycine loop is highly flexible and was observed in two distinct alternative conformations in the BTK-KD (amino acids 397 to 659 of SEQ ID NO: 2) crystal structure. One conformation of the β1 strand is similar to the conformation of the corresponding β1 strand in cAPK-KD, whereas the other conformation places residues T410-N412 of SEQ ID NO: 2 in a position that allows the triphosphate of ATP to bind BTK molecule A. A portion of the glycine loop is disordered in BTK molecule B that is related to molecule A by a

non-crystallographic two-fold axis. The adopted conformation of the invariant PTK residues D439-G441 (DFG) in BTK-KD (amino acids 397 to 659 of SEQ ID NO: 2) is consistent with the conformation of the same residues in the apo-IRK structure (19).

Figure 4 and Figure 5 are computer images showing the non-inhibitory (BTK) (Figure 4) and inhibitory (IRK) (Figure 5) conformations of the A-loop.

Unique non-inhibitory conformation of the activation loop in BTK kinase domain

Although it is highly mobile (B-factors of 30-40 $Å^2$), the "activation loop" (A-loop) of BTK-KD, except for residues S553-G556 of SEQ ID NO: 2, is visible within the electron density map. The A-loop of the BTK-KD is structurally very similar to the A-loop in the phosphorylated LCK-KD and the peptide substrate-bound IRK-KD structures, which contain a phosphorylated tyrosine residue (see Figure 3, IRK is not shown). R544, E445 and Y551 of SEQ ID NO: 2 are well defined in electron densities, as shown in the 2Fo-Fc electron density map (Figure 2, contoured at 1.0 σ and shown in stereo view). Based on the distance and geometry in the refined structure, the hydroxyl group of Y551 of SEQ ID NO: 2 interacts with R544 (SEQ ID NO: 2), S553 (SEQ ID NO: 2), and a water molecule via hydrogen bonds, and this group possibly interacts electrostatically with the nearby R520 residue (SEQ ID NO: 2). The aromatic ring of Y551 (SEQ ID NO: 2) has van der Waals contacts with V546 and F574 (SEQ ID NO: 2). Y551 (SEQ ID NO: 2) of the A-loop of the BTK-KD (SEQ ID NO: 2) is not phosphorylated but it interacts with R544 as is the case for the phospho-IRK and phospho-LCK structures. The structural difference is that the unphosphorylated Y551 (SEQ ID NO: 2) in the A-loop of the BTK-KD (SEQ ID NO: 2) interacts with R544 via a hydroxyl group rather than through a phosphate (see Figure 6). The crystal structure of the BTK-KD (amino acids 397 to 659 of SEQ ID NO: 2) indicates that the A-loop is essentially in a closed noninhibitory conformation (Figures 3 and 4). Both crystal structures were first superimposed and shown separately in the same orientation with the A-loops highlighted as tubes. Neither of the activation tyrosines is phosphorylated in crystal structures. These figures were prepared with GRASP (41). Hence, only minor structural adjustments would be expected for Y551 (SEQ ID NO: 2) and the surrounding residues upon Y551 (SEQ ID NO: 2) phosphorylation. Similarly, only minor structural changes in the orientation of the loop residues G556-P560 (SEQ ID

NO: 2) would be expected upon substrate binding. A similar active conformation of the A-loop has also been observed in the crystal structures of the recently reported checkpoint (CHK1) kinase (19), and CHK1-like phosphorylase kinase (PHK) (32, 55), in which the catalytic core is constitutively active. This unique conformation of the A-loop of the unphosphorylated BTK-KD supports a novel molecular mechanism for its initial activation (Figures 6 and 7).

The A-loop of kinase domains of PTKs and protein serine kinases (PSKs) usually serves as a negative regulator of kinase activity by blocking ATP binding and/or substrate peptide binding (20). Several protein kinases, including IRK, calmodulin-dependent protein kinase II, myosin light-chain kinase and protein kinase C, have a pseudosubstrate sequence within the A-loop that sterically blocks the access to the catalytic cleft by a substrate peptide (see review (23)). In the apo-IRK structure, the A-loop involving the Y551 (SEQ ID NO: 2) -equivalent tyrosine residue behaves as a substrate peptide mimic and sterically blocks access to the active site (Figure 5) (18, 19). Similarly, the A-loop in the inactive c-SRC, although different from that in apo-IRK, also hinders peptide binding and blocks access to the active site (Figure 3) (70, 72). The auto-inhibition mechanism illustrated in the apo-IRK structure was thought to be applicable to BTK as well (52). However, a close examination of the BTK-KD (amino acids 397 to 659 of SEQ ID NO: 2) crystal structure reveals that Y551 (SEQ ID NO: 2) is not near the active site residue D521 (Figures 3 and 4). Contrary to the expectations, the catalytic cleft of the BTK-KD (amino acids 397 to 659 of SEQ ID NO: 2) is not occluded by the A-loop or by any other portion of the KD. The conformation of A-loop in unphosphorylated BTK-KD structure is very similar to the active conformation of phosphorylated LCK-KD and hence does not limit substrate access to the active site.

Activation of BTK by transphosphorylation of the activation loop tyrosine residueY551

In a typical protein kinase structure, the beginning and end of the loop from helix αC to β4 and the linker loop between the lobes (N and C) act as hinge points (22). Correspondingly, two critical structural components that are associated with the active state conformation include the closure of the two lobes and the position of helix αC relative to the N-lobe. The two lobes (N (amino acids 397 to 475 of SEQ ID NO: 2) and C (amino acids 397 to 659 of SEQ ID NO: 2)) in the

BTK (SEQ ID NO: 2) structure adopt a closed conformation. A nearly identical conformation was observed for the two BTK-KD (amino acids 397 to 659 of SEQ ID NO: 2) molecules that are related by a 2-fold non-crystallographic symmetry and have different molecular packing. This suggests that the apo-BTK kinase domain favors a closed/active conformation. However, the distance of helix αC from the active site is larger in BTK-KD than it is in IRK and c-APK ternary complex structures. The distance between E445 and K430 is 10.2 Å in BTK-KD (amino acids 397 to 659 of SEQ ID NO: 2), and the corresponding distances in IRK and c-APK ternary complexes are approximately 3 Å.

K430 and E445 of SEQ ID NO: 2 are two invariant residues in the structural superfamily of protein kinases (15). Even very conservative mutations of these residues in BTK-KD (amino acids 397 to 659 of SEQ ID NO: 2)such as K430R and E445D have been associated with severe XLA (66). Mutations of the less-conserved R544 (SEQ ID NO: 2) residue are also associated with severe XLA (47). The location of the E445 (SEQ ID NO: 2)-equivalent residue relative to the K430 (SEQ ID NO:2)-equivalent residue and the location of the E445 (SEQ ID NO: 2)-equivalent residue relative to the ATP triphosphate serve as indicators of whether helix αC is in a favorable position for catalysis (70) (Figures 6 and 7). In the active KD structures such as those of the peptide-bound cAPK-KD and IRK-KD or phosphorylated LCK-KD (Figure 6), the E445 (SEQ ID NO: 2)-equivalent residues are associated with the K430 (SEQ ID NO: 2)-equivalent residue and the ATP triphosphate either directly by hydrogen bonding, or indirectly through a medium of molecules such as water or Mg (Figure 6). The C-terminal oxygen atoms of E445 (SEQ ID NO: 2) in the BTK structure (amino acids 397 to 659 of SEQ ID NO: 2) are 10.2 Å away from the K430 terminal atom. E445 (SEQ ID NO: 2) is hydrogen bonded to R544 (SEQ ID NO: 2), suggesting that R544 may play a regulatory role in preventing E445 from relocating to the active site and may hinder hydrogen bond formation with K430 (SEQ ID NO: 2).

This unique structural arrangement strongly suggests a novel molecular mechanism of activation by Y551 phosphorylation (Figure 7). Upon phosphorylation of Y551 (SEQ ID NO: 2), R544 (SEQ ID NO: 2) may be more engaged in the interaction with the phosphate group of P*Y551 and as a consequence, E445 (SEQ ID NO: 2) could be released to relocate to the active site and form a hydrogen bond with K430 (SEQ ID NO: 2). Helix αC in the BTK-KD

(amino acids 397 to 659 of SEQ ID NO: 2) structure has to be rotated by 20° from the pivot point at residue L452 (Figure 6). Therefore, the phosphorylation of Y551 (SEQ ID NO: 2) may activate BTK (SEQ ID NO: 2) by disengaging R544 (SEQ ID NO: 2) and E445 (SEQ ID NO: 2), which consequently enables E445 to take part in the catalytic reaction, as illustrated in Figure 7.

This unique regulatory inhibition of BTK (SEQ ID NO: 2) by R544 differs from the regulatory inhibition of c-SRC by SH3, in which the salt bridge formation between E310 (equivalent to E445 (SEQ ID NO: 2)) and K295 (equivalent to K430 (SEQ ID NO: 2)) is prevented by the binding of the c-SRC SH3 domain to the proline-rich linker region between SH2 and catalytic domains (17, 69); it also differs from the mechanism of CDK2, in which the relocation of helix αC is stabilized with the help of binding with cyclin. In summary, the activation of BTK (SEQ ID NO: 2) by Y551 phosphorylation likely involves an exchange of hydrogen-bonded pairs from E445/R544 to E445/K430, which can occur in concert with the phosphorylation of Y551 and subsequent relocation of helix αC.

The BTK Y551F mutant was reported to abrogate BTK autophosphorylation (33). Others observed that Y551F mutation causes a 90% reduction of LYN-mediated enhancement of both BTK tyrosine phosphorylation and kinase activity (52). A phenylalanine residue cannot engage in hydrogen-bonding interactions that link Tyr 551 (SEQ ID NO: 2) to R544 (SEQ ID NO: 2) and thus the conformation of the activation loop bearing this mutation may only partially resemble the internally bound inhibitory configuration. On the other hand, the Y551F mutant loses the ability to be phosphorylated and based on our proposed mechanism cannot release E445 to the active site. In contrast, the Y551 (SEQ ID NO: 2)-equivalent residue of c-SRC when mutated to phenylalanine was predicted to unlock the inhibitory "A helix" and actually activate the kinase activity (70). These observations point to an interesting difference between BTK and the kinase proteins of the SRC family. The X-ray crystal structure of the BTK-KD (amino acids 397 to 659 of SEQ ID NO: 2) revealed that neither Y551 nor Y545, the other tyrosine residue of the A-loop, reside in the catalytic site. This finding strongly supports the notion that BTK is activated by a trans-phosphorylation mechanism (via intermolecular interaction) at Y551 as suggested in previous experiments with LYN (43, 52, 68), rather than a cis-phosphorylation mechanism.

Example 8: BTK-KD Substrate Binding Model

To further elucidate the structural basis of the BTK activation, a P*Y551-BTK/ATP+Mg/peptide ternary complex model was constructed (Figures 8 and 9). The model was obtained by adjusting the coordinates of the BTK-KD (amino acids 397 to 659 of SEQ ID NO: 2) structure by first rotating helix αC of BTK-KD to emulate the phospho-LCK structure and then adjusting the glycine loop to accommodate the substrates, based on the IRK ternary complex structure. An analysis of this new BTK-KD model and the BTK-KD (amino acids 397 to 659 of SEQ ID NO: 2) crystal structure revealed no major steric clashes in the path of the 20° rotation between helix αC and the rest of the BTK-KD molecule.

Figure 8 shows a computer image of a backbone model of phosphorylated BTK-KD (amino acids 397 to 659 of SEQ ID NO: 2) associated with ATP, Mg^{++} and the substrate Igα peptide. Specifically, Mg^{++} ions (spheres), ATP triphosphate and peptide substrate are shown in contact via hydrogen bond or electrostatic interaction (thin lines). The in-line phosphoryl transfer mechanism for BTK is proposed (indicated by arrows). Figure 9 shows a space-filling model of this phospho-BTK-KD/ATP/Mg^{++}/Igα peptide complex.

Structural features of the substrate binding site of BTK

The peptide binding loop (S557-P560) of BTK-KD (amino acids 397 to 659 of SEQ ID NO: 2) adopts a β strand conformation and presumably interacts with the substrate peptide in an anti-parallel manner, as observed in the IRK, PHK and cAPK ternary structures. A peptide hexamer derived from an ITAM motif of Igα (NLY*EGL), a known physiologic substrate of BTK (46), has been modeled into the peptide binding site of BTK-KD using the IRK ternary structure as a template (shown in Figures 8 and 9).

The peptide substrate-binding site of BTK-KD (amino acids 397 to 659 of SEQ ID NO: 2) is a shallow groove 16 Å long on the protein surface and can accommodate the binding of a portion of the target peptide substrate between the P-2 to P+3 positions. The first half of the binding site is a circular region of 5.8 Å in radius, centered around the P-1 carbonyl group. This region can bind the residues from P-2 to P, with the side chain groups of the P tyrosine and the P-1 residue being surrounded by the BTK-KD (amino acids 397 to 659 of SEQ ID NO: 2) residues

(Figures 8 and 9). The remaining atoms of the residues from P-2 to P are mostly exposed to the solvent environment.

An "enclosed" binding site is generally highly selective for peptide substrates whereas an "open" binding site is not. The cAPK crystal structure revealed an enclosed and negatively charged binding site for the Arg (P-1) residue (39). The PHK crystal structure demonstrated an enclosed polar binding site for Gln (P-2) formed by the P+1 loop which contains a Ser, Thr and Pro (32). In contrast, the BTK complex model suggests a half-buried and spacious P-1 binding site like the substrate binding site in IRK (18) (Figure 9). However, L483 of BTK (SEQ ID NO: 2) contributes to a preference for a hydrophobic P-1 residue whereas K1085 in IRK can be associated with a preference for a negatively charged P-1 residue.

SYK has an asparagine residue corresponding to L483 (SEQ ID NO: 2) and preferentially selects an aspartic residue for the P-1 residue over other types of residues (e. g. SYK selects a DYE motif (54)). Overall, the aliphatic portion of R525 of SEQ ID NO: 2 and the side chain groups of L483, C481, R487 and M596 of SEQ ID NO: 2 likely define the P-1 binding subsite. The sequence alignment of these residues with those of SRC family PTKs indicates a similar binding environment and therefore a similar recognition pattern for the P-1 position. c-SRC, BLK and LYN all preferentially select a leucine or isoleucine as the P-1 residue (54). Similarly, BTK (SEQ ID NO: 2) is also likely to preferentially select a leucine or isoleucine as the P-1 residue, which is consistent with the notion that LY(223)D is a more favored BTK autophosphorylation site than EY(551)TSS (52).

The side chain group of the tyrosine targeted for phosphorylation on the substrate peptide is in contact with P560 (SEQ ID NO: 2), R525 (SEQ ID NO: 2), D521 (SEQ ID NO: 2), γ-phosphate and possibly with the side chain groups of Q412 and K558 (SEQ ID NO: 2). The enclosed binding environment is consistent with a highly discriminating binding pocket for the P tyrosine.

The Glu (P+1) residue in BTK (SEQ ID NO: 2) is close to F559 and interacts with N603. Residues larger than Glu can potentially interact with residue S604 (SEQ ID NO: 2). Previous crystal structures for PTK kinase domains have not shown a specific and enclosed binding site for the P+1 residue, as well as in this current BTK-KD (amino acids 397 to 659 of SEQ ID NO: 2) crystal structure.

Therefore the selection for the P+1 residue is unlikely to be strict. However, in light of the differences for these three residues at the P+1 position, BTK (SEQ ID NO: 2) is more similar to SRC family PTKs than it is to IRK or SYK. Residues that correspond to F559, N603 and S604 of BTK (SEQ ID NO: 2) are specified in parentheses: IRK (L,N,E), SYK (K,G,S), SRC (F,N,R), LYN (F,N,A), BLK (F,N,P).

Our model is consistent with the phosphoryl transfer mechanism of an in-line nucleophilic attack. Specifically, D445 (SEQ ID NO: 2), K430 (SEQ ID NO: 2), a Mg ion, and α- and β-phosphate groups form a network of electrostatic interactions and hydrogen bonds presumably to align the ATP molecule in a conformation suitable for reaction (Figure 8). D539 (SEQ ID NO: 2) and the second Mg ion orient the γ-phosphate group for the in-line attack. The model indicates that the hydroxyl group of the P tyrosine forms a hydrogen bond with D521 (SEQ ID NO: 2), consistent with the activation mechanism in which the attacking group is deprotonated by an aspartic acid residue.

Example 9: Design of Modulators of BTK

To design specific modulators of BTK (SEQ ID NO: 2), the crystal structure coordinates for the kinase domain of BTK (amino acids 397 to 659 of SEQ ID NO: 2) are used to model, predict, and identify specific ligands for modulating (inhibiting or stimulating) BTK activity.

K_i values that quantitate predicted binding interactions between the inhibitor and residues in the kinase domain of BTK (amino acids 397 to 659 of SEQ ID NO: 2) are estimated, for example as described in Mahajan, et al. 1999 (34). Each ligand is individually modeled into the catalytic site of the BTK kinase domain (amino acids 397 to 659 of SEQ ID NO: 2) using an advanced docking procedure (34, U.S. Patent No. 6,294,575, issued September 25, 2001 and U.S. Patent No. 6,303,652, issued October 16, 2001). The various docked positions of each ligand are qualitatively evaluated using a scoring procedure and consequently compared with the IC_{50} values of the ligands in cell-free BTK inhibition assays. The interaction scores, calculated K_i values, and measured IC_{50} values for each ligand complexed with BTK (amino acids 397 to 659 of SEQ ID NO: 2) is evaluated.

Apoptosis Assays

BTK inhibition assays include assays of cellular apoptosis induced by BTK (SEQ ID NO: 2). To induce apoptosis, cells were treated with an agonistic anti-Fas/APO-1 antibody (Biosource International, Camarillo, CA, lot. 04/1295) at 0.1 μg/ml, 0.5 μg/ml, or 1.0 μg/ml final concentrations. MC540 binding (as an early marker of apoptosis) and PI permeability (as a marker of advanced stage apoptosis) were simultaneously measured in DT-40 cells 24 hours after exposure to anti-Fas antibody as previously described (59). Whole cells were analyzed with a FACStar Plus flow cytometer (Becton Dickinson, San Jose, CA). All analyses were done using 488 nm excitation from an argon laser. MC540 and PI emissions were split with a 600 nm short pass dichroic mirror and a 575 nm and pass filter was placed in front of one photomultiplier tube to measure MC540 emission and a 635 nm band pass filter was used for PI emission.

To detect apoptotic fragmentation of DNA, DT-40, NALM-6-UM1, and RAMOS-1 cells were harvested 24 hours after exposure to anti-Fas. DNA was prepared from TRITON-X-100 lysates for analysis of fragmentation (59, 60). Cells were lysed in hypotonic 10 mmol/L TRIS-HCl (pH 7.4), 1 mmol/L EDTA, 0.2% TRITON-X-100 detergent; and subsequently centrifuged at 11,000 x g. To detect apoptosis-associated DNA fragmentation, supernatants were electrophoresed on a 1.2% agarose gel, and the DNA fragments were visualized by ultraviolet light after staining with ethidium bromide.

Example 910: Mapping XLA Mutations

Although a homology model of BTK-KD (amino acids 397 to 659 of SEQ ID NO: 2) is useful for providing the structural basis of XLA-causing mutations, a BTK-KD (amino acids 397 to 659 of SEQ ID NO: 2) crystal structure provides a more accurate interpretation, especially considering that the two-lobe conformation among kinases and the geometry of active site could vary significantly. Most of known XLA-causing missense mutations are listed in Table **3 4**, together with structural consequences of these mutations. Many of the XLA mutations map to the sites known to be important for the mechanism of BTK-KD (amino acids 397 to 659 of SEQ ID NO: 2) activation described above (see Figure 10). Figure 10 maps X-linked agammaglobulinaemia (XLA) related mutations on the crystal structure of the BTK kinase domain (amino acids 397 to 659 of SEQ ID NO: 2), shown in stereo

view. Several XLA mutations involve residues that are highly conserved and may be part of the catalysis machinery. Some XLA mutations involve other important active site residues. Many XLA mutations involve the residues, which stabilize the hydrophobic core structure of the C-lobe domain. Other XLA mutations involve the residues of the lobe linker region and the peptide substrate-binding region. This figure was prepared with the INSIGHT II program suite (1997, Molecular Simulations, Inc., San Diego, CA).

TABLE 3 4

XLA associated BTK missense mutations

BTK mutation associated with XLA		**Structural Position and Function of Involved Residue**	**Structural Conseq-uences**
*Residue#	Amino acid		
408	L→P	maintain the beta conformation of the αl strand	A, indirectly
414	G→R	highly conserved residue, backbone forms a hydrogen bond with the β phosphate of ATP	A
418	Y→H	maintain the local hydrophobic structural stability near the domain hinge region	A, indirectly
429	I→N	in a hydrophobic cluster and maintain the natural curvature of the N-lobe β sheet	B
430	K→E K→R	invariant residue of PTK family, align ATP via interaction with the α phosphate	C
445	E→D	invariant residue of PTK family, align ATP via interaction with the β phosphate	C
462	G→D G→V	on the β4 strand and the interface with β-sheet and helix C	E
476	Y→D	close to adenine base of ATP	D
477	M→R	close to adenine base of ATP	D
502	C→F C→W	on helix E, interact with F583 and M587 in a compact hydrophobic cluster	B
504	D→V	ion pair with K456, near the hinge region of helix C	D
506	C→R C→Y	on helix E, interact with F583(helix F) and the carbonyl groups of 644 and 502	B
508	A→D	on helix E, near the hinge region of helix C	D
509	M→I M→V	interact with I522 and V537 in a compact hydrophobic cluster	B
512	L→P L→Q	near the side chains of L457, L452 and F517, M509 in a compact hydrophobic cluster	B
518	L→R	close to V546, F574 and Y551 in a hydrophobic cluster	B+E
520	R→Q	conserved in all "RD" kinases, interacts with the nearby activation Y551, stabilizing the phospho-tyrosine	B+E
521	D→G D→H D→N	invariant residue of PTK family, activation of the nucleophilic attacking hydroxyl group of the target residue (tyrosine in BTK) by deprotonation	C
525	R→P	alignment and stabilization of the γ-phosphate	A

* Amino acid residue of SEQ ID NO: 2

	R→Q	during phosphoryl transfer process	
526	N→K	invariant residue of PTK family, coupled with D539 to align the γ-phosphate of ATP	A
535	V→F	interact with L665	D
542	L→P	near the highly conserved DFG motif which adopts two different conformations during catalytic process	*D*
544	R→K R→G	form a hydrogen bond with E445 in a nonproductive conformation	see text
559	F→S	in the P+1 substrate binding pocket	*F*, P+1
562	R→P R→W	on a helix turn starting from P560 to S564 in the protein substrate binding site	F
563	W→L	hydrophobic interaction with A523 and is part of protein substrate binding pocket	*F*
567	E→K	ion pair with R641 and thus contribute to the interaction between helix EF and helix H or I.	*B*
569	L→P	on helix EF	*B*
578	S→Y	on helix F, hydrogen bonded with the 575 amide near the activation loop	*B*
581	W→R	on helix F, hydrophobic interaction with W634 in a compact hydrophobic cluster	*B*
582	A→V	near the 522 carbonyl group and D521	*A+E'*
583	F→S	see 506	*B*
587	M→L	on helix F, see 502	*B*
589	E→D E→G	on helix F, see 506	*B*
592	S→P S→Y	forms a hydrogen bond with the 595 amide	*B*
594	G→E G→R	near R487 which forms part of the P-1 binding pocket	*F*, P-1
597	P→T	buried near M596 which forms part of the P-1 binding pocket	*F*, P-1
598	Y→C	interact with F601, L616 and T606 in a compact hydrophobic cluster	B
606	T→P	on the inward face of helix G, see 598	*B*
607	A→D	on helix G, mostly exposed	*X*
613	G→D	near R615	*X*
616	L→F	on helix G, interact with W634, Y598 and W588 in a compact hydrophobic cluster	*B*
619	P→A P→/S/T	on the inward face of helix G and close to W588, S592 and A622	*B*
622	A→P	interact with 619, see 619	*B*
626	V→G	form a hydrophobic cluster on the inward face of helix H and close to Y591	*B*
630	M→K M→T	on the inward face of helix H, interacts with W634 and W588	*B*

633	C→Y	on the inward face of helix H in a compact hydrophobic cluster	B
641	R→C R→H	on helix H and pair with E567, see 567	*B*
644	F→L F→S	on the inward face of helix I and in a hydrophobic cluster	*B*
647	L→R	on the inward face of helix I and close to C633 and F583	*B*
652	L→P	exposed	*X*

* Missense mutations were obtained from *BTKbase*, a mutation database for X-linked agammaglobulinemia (see website: protein.uta.fi/BTKbase/btkpub.html); *A*: affect the ATP binding; *B*: affect local structural stability; *C*: disrupt interaction with E445 and affect the catalytic reaction; *D*: interfere with domain "breathing"; *E*: interfere with the activation process; *E'*: affect helix C and activation; *F*: change sequence selection preference; *X*: no foreseeable effect on kinase activity: P-1: affect the P-1 binding pocket; P+1: affect the P+1 binding pocket.

Observations involving R544K/G and K430R mutations (Table 3) are intriguing. An arginine residue is different from a lysine residue in side chain length as well as hydrogen bonding capability and interactions with phosphate and/or glutamic acid residues. These differences may adversely affect the binding of ATP to the catalytic domain of BTK R544K/G (Table 3). The R544G mutant may not be able to stabilize the phosphorylated Y551 (SEQ ID NO: 2) and may consequently destabilize the A-loop, the position of which is sensitive for correct alignment of peptide substrate binding. On the other hand, R544G (Table 3) would be expected to unlock E445 (SEQ ID NO: 2) and would probably trigger part of the activation process as discussed earlier in this paper. The effect of R544K mutation (Table 3) on BTK (SEQ ID NO: 2) kinase activity is less certain because the R544-equivalent residues vary in different PTKs. The BTK (SEQ ID NO: 2) structure suggests that R544K (Table 3) is unlikely to abolish the kinase activity entirely.

R520 (SEQ ID NO: 2) is not entirely conserved in the protein kinase superfamily but is present in all "RD" kinases that require activation by phosphorylation (23). Notably, the R520 (SEQ ID NO: 2) -equivalent residue in IRK was found to be mutated (R1131N) in patients with non-insulin-dependent diabetes mellitus (NIDDM) (1). The side chain of R520 is close to Y551 in the BTK-KD (amino acids 397 to 659 of SEQ ID NO: 2) crystal structure. A survey of the equivalent residue in the "RD" kinase structures revealed that the R520 (SEQ ID NO: 2) -equivalent residue is close to a phosphate or a carboxylate group and apparently plays a role in stabilizing the phospho-tyrosine/Ser/Thr. The hot-spot mutation R520Q (Table 3) certainly changes the interaction pattern with P*Y551 and a glutamine residue is much less likely to be associated with a phosphate group than an arginine residue (8). Thus, the R520Q (Table 3) mutant probably would have a destabilized activation loop.

XLA-associated BTK mutations involving the N-lobe of the kinase domain (amino acids 397 to 659 of SEQ ID NO: 2) are less frequent than those involving the C-lobe (amino acids 397 to 659 of SEQ ID NO: 2) (Figure 10 and Table 3 4). G414, L408, Y418, and I429 (SEQ ID NO: 2) were identified as "mutation hot spots" in XLA patients. Notably, residue G414 (SEQ ID NO: 2) which is highly conserved as a glycine (or less likely, small residues like alanine) is located at the beginning of the β2 strand and is right on top of the triphosphate group of ATP where its backbone forms a hydrogen bond with the oxygen atom of the γ-phosphate. At this

position, a large side chain substitution such as the G414R (SEQ ID NO: 2) mutation would dramatically limit the loop flexibility that may be required to accommodate ATP and subsequently release ADP. With the arginine substitution, neither the hydrogen bonding nor the ATP binding conformation would be optimal.

In the crystal structure of the IRK ternary complex, the β1-β2 loop adopts a common β turn type III, in which the i+3 position, which corresponds to G414 in BTK (SEQ ID NO: 2), is predominantly occupied by a flexible glycine residue G1008 which allows the defined conformation and is presumably necessary for correctly placing the ATP phosphate in the BTK (SEQ ID NO: 2) catalytic site. A G1008V mutation in IRK has been found in patients with NIDDM (1). A more dramatic G414R substitution (Table 3) in BTK (SEQ ID NO: 2) is likely to alter the conformation to become incompatible with the correct alignment of ATP for catalysis.

Modeling studies indicate that the XLA-associated mutations W563L, P597T, F559S and R562 (Table 3) can be directly or indirectly involved in the peptide substrate binding. W563 of SEQ ID NO: 2 is situated between P597 and A523 of SEQ ID NO: 2, the latter of which is near the center of the active site. W563L mutation (Table 3) may alter the conformation of the peptide subsite and has been identified in patients with XLA. P597 of SEQ ID NO: 2 is relatively distant from the central region of the active site but the side chain of P597 of SEQ ID NO: 2 is totally buried behind the nearby residues including M596 of SEQ ID NO: 2, which forms part of the P-1 binding pocket (see Figure 9). The nearest atom pairs between W563 and P597 or A523 of SEQ ID NO: 2 are 3.7 Å away. The three residues are packed against each other as the core part of the substrate peptide-binding site. Clearly, the P597T mutation (Table 3) would impair substrate binding. By comparison, the F559S mutation may change the selection preference of the binding region for the P+1 position (Table 3) (see Figure 9). The side chain of R562 of SEQ ID NO: 2 forms a network of hydrogen bonds with N603, which is a part of the P+1 binding pocket, and T606 of SEQ ID NO: 2, which is connected to the main chain carbonyl group. The R562P mutation (Table 3) can be expected to alter the helical turn due to the rigid proline residue and thereby change the local conformation including that of the important PTK invariant P-site residue P560 of SEQ ID NO: 2. The R1174N mutant (corresponds to a mutation of R562 of SEQ ID NO: 2) in IRK has been identified in NIDDM patients.

Remarkable insights were gained by mapping the XLA-associated missense mutations of the C-lobe (amino acids 397 to 659 of SEQ ID NO: 2) onto the BTK-KD (amino acids 397 to 659 of SEQ ID NO: 2) crystal structure. Most of these mutations on the C-lobe are concentrated on the inward face of helices and loops (see residues in Figure 10). According to our analysis, the majority of the side chains are at least half-buried, suggesting that these mutations may destabilize the C-lobe of the kinase domain (amino acids 397 to 659 of SEQ ID NO: 2) by altering its interactions with neighboring residues (see also Table 3 4). The mutations include S578Y, W581R, A582V, F583S, M587L, E589D/G and S592P (Table 3) on both sides of helix αF that is flanked by other helices. The inward sides of helices αE, αG, and αI, appear to be most susceptible to XLA-causing mutations (see Figure 10). The inward face of loops located between the helices of the C-lobe (amino acid residues 479 to 659 of SEQ ID NO: 2), although lying exposed on the protein surface, are also susceptible to mutation. L652P (Table 3) is an exception in that its side chain occurs on the protein surface. Therefore, the functional implications of this mutation should be interpreted with caution.

All publications, patents, and patent documents are incorporated by reference herein, as though individually incorporated by reference. The invention has been described with reference to various specific and preferred embodiments and techniques. However, it should be understood that many variations and modifications may be made while remaining within the spirit and scope of the invention.

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TABLE 4 5*

Atom Number	Atom Type	Amino Acid Residue		X	Y	Z	Occ.	Temp Factor	
ATOM 1	CB	ILE	397	39.984	4.826	17.892	1.00	26.05	BTKA
ATOM 2	CG2	ILE	397	41.212	3.952	17.664	1.00	28.70	BTKA
ATOM 3	CG1	ILE	397	39.927	5.294	19.346	1.00	21.76	BTKA
ATOM 4	CD	ILE	397	38.668	6.044	19.704	1.00	19.11	BTKA
ATOM 5	C	ILE	397	41.382	6.663	16.890	1.00	28.45	BTKA
ATOM 6	O	ILE	397	42.042	6.591	15.857	1.00	27.84	BTKA
ATOM 7	N	ILE	397	39.699	5.634	15.537	1.00	31.08	BTKA
ATOM 8	CA	ILE	397	39.996	6.043	16.938	1.00	27.95	BTKA
ATOM 9	N	ASP	398	41.833	7.254	17.988	1.00	29.89	BTKA
ATOM 10	CA	ASP	398	43.142	7.879	17.991	1.00	30.58	BTKA
ATOM 11	CB	ASP	398	42.982	9.399	17.868	1.00	27.36	BTKA
ATOM 12	CG	ASP	398	44.227	10.080	17.336	1.00	26.98	BTKA
ATOM 13	OD1	ASP	398	45.346	9.607	17.635	1.00	23.87	BTKA
ATOM 14	OD2	ASP	398	44.078	11.087	16.601	1.00	23.63	BTKA
ATOM 15	C	ASP	398	43.966	7.548	19.230	1.00	33.13	BTKA
ATOM 16	O	ASP	398	43.564	7.860	20.350	1.00	34.18	BTKA
ATOM 17	N	PRO	399	45.080	6.820	19.050	1.00	36.49	BTKA
ATOM 18	CD	PRO	399	45.461	6.040	17.861	1.00	38.51	BTKA
ATOM 19	CA	PRO	399	45.938	6.472	20.187	1.00	36.60	BTKA
ATOM 20	CB	PRO	399	46.941	5.494	19.573	1.00	34.91	BTKA
ATOM 21	CG	PRO	399	46.157	4.851	18.479	1.00	38.91	BTKA
ATOM 22	C	PRO	399	46.625	7.765	20.581	1.00	35.91	BTKA
ATOM 23	O	PRO	399	47.165	8.454	19.718	1.00	35.42	BTKA
ATOM 24	N	LYS	400	46.574	8.114	21.861	1.00	36.75	BTKA
ATOM 25	CA	LYS	400	47.189	9.349	22.325	1.00	33.61	BTKA
ATOM 26	CB	LYS	400	46.860	9.604	23.800	1.00	34.79	BTKA
ATOM 27	CG	LYS	400	47.406	10.924	24.332	1.00	32.92	BTKA
ATOM 28	CD	LYS	400	47.052	11.127	25.795	1.00	32.83	BTKA
ATOM 29	CE	LYS	400	45.589	11.506	25.982	1.00	33.63	BTKA
ATOM 30	NZ	LYS	400	45.298	12.915	25.566	1.00	32.25	BTKA
ATOM 31	C	LYS	400	48.698	9.448	22.083	1.00	31.96	BTKA
ATOM 32	O	LYS	400	49.510	9.153	22.958	1.00	27.95	BTKA
ATOM 33	N	ASP	401	49.059	9.828	20.863	1.00	32.35	BTKA
ATOM 34	CA	ASP	401	50.453	10.014	20.493	1.00	31.87	BTKA
ATOM 35	CB	ASP	401	50.805	9.258	19.196	1.00	32.78	BTKA
ATOM 36	CG	ASP	401	49.823	9.521	18.057	1.00	34.30	BTKA
ATOM 37	OD1	ASP	401	49.422	8.542	17.390	1.00	31.33	BTKA
ATOM 38	OD2	ASP	401	49.466	10.692	17.811	1.00	34.83	BTKA
ATOM 39	C	ASP	401	50.645	11.520	20.347	1.00	29.99	BTKA
ATOM 40	O	ASP	401	51.112	12.016	19.321	1.00	28.60	BTKA
ATOM 41	N	LEU	402	50.212	12.238	21.378	1.00	30.44	BTKA
ATOM 42	CA	LEU	402	50.307	13.686	21.416	1.00	32.58	BTKA
ATOM 43	CB	LEU	402	48.911	14.310	21.538	1.00	29.13	BTKA
ATOM 44	CG	LEU	402	47.769	13.911	20.596	1.00	28.32	BTKA
ATOM 45	CD1	LEU	402	47.220	12.552	20.969	1.00	26.12	BTKA
ATOM 46	CD2	LEU	402	46.662	14.931	20.708	1.00	26.92	BTKA
ATOM 47	C	LEU	402	51.150	14.087	22.624	1.00	35.40	BTKA
ATOM 48	O	LEU	402	51.460	13.254	23.476	1.00	36.97	BTKA
ATOM 49	N	THR	403	51.538	15.356	22.681	1.00	36.15	BTKA
ATOM 50	CA	THR	403	52.330	15.864	23.793	1.00	35.21	BTKA
ATOM 51	CB	THR	403	53.584	16.641	23.296	1.00	35.16	BTKA
ATOM 52	OG1	THR	403	53.287	17.328	22.073	1.00	36.34	BTKA

* The coordinates correspond to the crystal structure of the polypeptide sequence of BTK-KD (amino acids 397 to 659 of SEQ ID NO: 2)

Atom Number	Atom Type	Amino Acid Residue		X	Y	Z	Occ.	Temp Factor	
ATOM	53	CG2	THR 403	54.745	15.688	23.072	1.00	33.51	BTKA
ATOM	54	C	THR 403	51.448	16.724	24.705	1.00	35.29	BTKA
ATOM	55	O	THR 403	50.473	16.214	25.266	1.00	34.77	BTKA
ATOM	56	N	PHE 404	51.761	18.014	24.834	1.00	32.58	BTKA
ATOM	57	CA	PHE 404	50.985	18.918	25.683	1.00	32.99	BTKA
ATOM	58	CB	PHE 404	51.060	18.457	27.151	1.00	33.57	BTKA
ATOM	59	CG	PHE 404	49.973	19.023	28.034	1.00	36.18	BTKA
ATOM	60	CD1	PHE 404	50.063	20.317	28.541	1.00	36.37	BTKA
ATOM	61	CD2	PHE 404	48.873	18.248	28.383	1.00	35.88	BTKA
ATOM	62	CE1	PHE 404	49.076	20.828	29.383	1.00	36.13	BTKA
ATOM	63	CE2	PHE 404	47.881	18.750	29.224	1.00	36.02	BTKA
ATOM	64	CZ	PHE 404	47.982	20.041	29.726	1.00	36.27	BTKA
ATOM	65	C	PHE 404	51.559	20.327	25.551	1.00	30.92	BTKA
ATOM	66	O	PHE 404	52.748	20.484	25.275	1.00	28.05	BTKA
ATOM	67	N	LEU 405	50.710	21.341	25.706	1.00	31.51	BTKA
ATOM	68	CA	LEU 405	51.156	22.730	25.627	1.00	31.53	BTKA
ATOM	69	CB	LEU 405	51.175	23.239	24.183	1.00	32.59	BTKA
ATOM	70	CG	LEU 405	51.990	24.521	23.961	1.00	33.86	BTKA
ATOM	71	CD1	LEU 405	53.466	24.150	23.845	1.00	34.64	BTKA
ATOM	72	CD2	LEU 405	51.533	25.263	22.706	1.00	37.27	BTKA
ATOM	73	C	LEU 405	50.343	23.672	26.521	1.00	32.49	BTKA
ATOM	74	O	LEU 405	50.538	23.676	27.735	1.00	33.98	BTKA
ATOM	75	N	LYS 406	49.411	24.434	25.948	1.00	35.17	BTKA
ATOM	76	CA	LYS 406	48.630	25.387	26.742	1.00	36.21	BTKA
ATOM	77	CB	LYS 406	49.411	26.702	26.877	1.00	33.84	BTKA
ATOM	78	CG	LYS 406	50.477	26.685	27.960	1.00	33.94	BTKA
ATOM	79	CD	LYS 406	51.410	27.884	27.867	1.00	35.43	BTKA
ATOM	80	CE	LYS 406	52.445	27.713	26.760	1.00	37.40	BTKA
ATOM	81	NZ	LYS 406	53.438	26.632	27.055	1.00	35.32	BTKA
ATOM	82	C	LYS 406	47.182	25.679	26.303	1.00	37.77	BTKA
ATOM	83	O	LYS 406	46.588	24.939	25.512	1.00	39.12	BTKA
ATOM	84	N	GLU 407	46.629	26.752	26.873	1.00	35.20	BTKA
ATOM	85	CA	GLU 407	45.263	27.221	26.633	1.00	34.68	BTKA
ATOM	86	CB	GLU 407	45.105	28.626	27.220	1.00	34.04	BTKA
ATOM	87	CG	GLU 407	43.747	29.277	26.974	1.00	28.63	BTKA
ATOM	88	CD	GLU 407	43.628	30.632	27.624	1.00	23.09	BTKA
ATOM	89	OE1	GLU 407	44.594	31.415	27.557	1.00	19.69	BTKA
ATOM	90	OE2	GLU 407	42.570	30.912	28.213	1.00	19.52	BTKA
ATOM	91	C	GLU 407	44.833	27.253	25.178	1.00	34.30	BTKA
ATOM	92	O	GLU 407	45.664	27.386	24.283	1.00	38.04	BTKA
ATOM	93	N	LEU 408	43.523	27.209	24.957	1.00	33.77	BTKA
ATOM	94	CA	LEU 408	42.980	27.248	23.608	1.00	35.95	BTKA
ATOM	95	CB	LEU 408	43.335	25.958	22.888	1.00	35.53	BTKA
ATOM	96	CG	LEU 408	44.349	26.065	21.763	1.00	33.73	BTKA
ATOM	97	CD1	LEU 408	45.091	24.751	21.657	1.00	32.87	BTKA
ATOM	98	CD2	LEU 408	43.649	26.440	20.453	1.00	33.61	BTKA
ATOM	99	C	LEU 408	41.473	27.516	23.537	1.00	36.07	BTKA
ATOM	100	O	LEU 408	40.836	27.827	24.549	1.00	30.55	BTKA
ATOM	101	N	GLY 409	40.923	27.400	22.328	1.00	37.82	BTKA
ATOM	102	CA	GLY 409	39.509	27.647	22.086	1.00	42.67	BTKA
ATOM	103	C	GLY 409	38.531	26.929	23.000	1.00	43.77	BTKA
ATOM	104	O	GLY 409	38.872	25.926	23.621	1.00	44.19	BTKA
ATOM	105	N	THR 410	37.300	27.426	23.053	1.00	44.64	BTKA
ATOM	106	CA	THR 410	36.269	26.844	23.903	1.00	44.12	BTKA
ATOM	107	CB	THR 410	35.790	27.859	24.963	1.00	42.36	BTKA
ATOM	108	OG1	THR 410	36.859	28.760	25.285	1.00	38.07	BTKA
ATOM	109	CG2	THR 410	35.353	27.141	26.225	1.00	42.56	BTKA
ATOM	110	C	THR 410	35.056	26.429	23.076	1.00	45.63	BTKA

	Atom Number	Atom Type	Amino Acid Residue		X	Y	Z	Occ.	Temp Factor	
ATOM	111	O	THR	410	34.984	26.700	21.874	1.00	46.48	BTKA
ATOM	112	N	GLY	411	34.106	25.776	23.739	1.00	45.00	BTKA
ATOM	113	CA	GLY	411	32.882	25.326	23.104	1.00	43.61	BTKA
ATOM	114	C	GLY	411	31.968	24.888	24.228	1.00	42.95	BTKA
ATOM	115	O	GLY	411	32.438	24.681	25.347	1.00	42.15	BTKA
ATOM	116	N	GLN	412	30.682	24.697	23.946	1.00	41.91	BTKA
ATOM	117	CA	GLN	412	29.736	24.291	24.984	1.00	40.64	BTKA
ATOM	118	CB	GLN	412	28.300	24.300	24.452	1.00	40.22	BTKA
ATOM	119	CG	GLN	412	27.748	25.702	24.225	1.00	38.55	BTKA
ATOM	120	CD	GLN	412	26.335	25.717	23.663	1.00	34.81	BTKA
ATOM	121	OE1	GLN	412	25.732	26.780	23.514	1.00	33.50	BTKA
ATOM	122	NE2	GLN	412	25.799	24.545	23.354	1.00	28.18	BTKA
ATOM	123	C	GLN	412	30.050	22.969	25.692	1.00	37.36	BTKA
ATOM	124	O	GLN	412	29.342	22.585	26.627	1.00	36.95	BTKA
ATOM	125	N	PHE	413	31.060	22.248	25.214	1.00	34.84	BTKA
ATOM	126	CA	PHE	413	31.468	21.000	25.853	1.00	32.28	BTKA
ATOM	127	CB	PHE	413	31.890	19.942	24.825	1.00	33.34	BTKA
ATOM	128	CG	PHE	413	30.742	19.163	24.226	1.00	30.57	BTKA
ATOM	129	CD1	PHE	413	29.490	19.749	24.032	1.00	30.22	BTKA
ATOM	130	CD2	PHE	413	30.934	17.850	23.800	1.00	29.00	BTKA
ATOM	131	CE1	PHE	413	28.451	19.039	23.417	1.00	29.05	BTKA
ATOM	132	CE2	PHE	413	29.899	17.133	23.183	1.00	27.19	BTKA
ATOM	133	CZ	PHE	413	28.659	17.728	22.990	1.00	25.29	BTKA
ATOM	134	C	PHE	413	32.649	21.334	26.753	1.00	31.49	BTKA
ATOM	135	O	PHE	413	32.865	20.701	27.783	1.00	28.50	BTKA
ATOM	136	N	GLY	414	33.413	22.346	26.353	1.00	33.87	BTKA
ATOM	137	CA	GLY	414	34.562	22.763	27.134	1.00	36.54	BTKA
ATOM	138	C	GLY	414	35.623	23.439	26.288	1.00	38.54	BTKA
ATOM	139	O	GLY	414	35.372	23.843	25.144	1.00	37.26	BTKA
ATOM	140	N	VAL	415	36.800	23.604	26.883	1.00	38.40	BTKA
ATOM	141	CA	VAL	415	37.944	24.225	26.228	1.00	35.19	BTKA
ATOM	142	CB	VAL	415	38.859	24.900	27.286	1.00	33.66	BTKA
ATOM	143	CG1	VAL	415	39.567	23.841	28.118	1.00	33.58	BTKA
ATOM	144	CG2	VAL	415	39.851	25.858	26.639	1.00	29.68	BTKA
ATOM	145	C	VAL	415	38.735	23.136	25.499	1.00	33.93	BTKA
ATOM	146	O	VAL	415	38.348	21.961	25.515	1.00	33.38	BTKA
ATOM	147	N	VAL	416	39.821	23.544	24.845	1.00	33.13	BTKA
ATOM	148	CA	VAL	416	40.716	22.648	24.124	1.00	28.19	BTKA
ATOM	149	CB	VAL	416	40.608	22.849	22.570	1.00	27.16	BTKA
ATOM	150	CG1	VAL	416	39.236	22.466	22.080	1.00	24.50	BTKA
ATOM	151	CG2	VAL	416	40.838	24.282	22.184	1.00	21.15	BTKA
ATOM	152	C	VAL	416	42.138	22.937	24.628	1.00	25.73	BTKA
ATOM	153	O	VAL	416	42.344	23.904	25.354	1.00	25.11	BTKA
ATOM	154	N	LYS	417	43.100	22.079	24.298	1.00	27.45	BTKA
ATOM	155	CA	LYS	417	44.505	22.255	24.723	1.00	28.38	BTKA
ATOM	156	CB	LYS	417	44.875	21.266	25.838	1.00	30.82	BTKA
ATOM	157	CG	LYS	417	44.299	21.627	27.207	1.00	32.85	BTKA
ATOM	158	CD	LYS	417	44.889	22.936	27.747	1.00	32.78	BTKA
ATOM	159	CE	LYS	417	44.092	23.465	28.933	1.00	30.38	BTKA
ATOM	160	NZ	LYS	417	42.671	23.743	28.566	1.00	24.07	BTKA
ATOM	161	C	LYS	417	45.429	22.050	23.531	1.00	22.74	BTKA
ATOM	162	O	LYS	417	44.971	21.628	22.482	1.00	23.20	BTKA
ATOM	163	N	ALA	418	46.717	22.344	23.670	1.00	19.60	BTKA
ATOM	164	CA	ALA	418	47.625	22.172	22.532	1.00	19.78	BTKA
ATOM	165	CB	ALA	418	48.484	23.410	22.334	1.00	19.67	BTKA
ATOM	166	C	ALA	418	48.493	20.924	22.550	1.00	19.25	BTKA
ATOM	167	O	ALA	418	48.892	20.446	23.619	1.00	19.18	BTKA
ATOM	168	N	GLY	419	48.751	20.398	21.352	1.00	16.40	BTKA

	Atom Number	Atom Type	Amino Acid Residue		X	Y	Z	Occ.	Temp Factor	
ATOM	169	CA	GLY	419	49.570	19.210	21.176	1.00	14.78	BTKA
ATOM	170	C	GLY	419	49.886	18.994	19.704	1.00	14.35	BTKA
ATOM	171	O	GLY	419	49.350	19.692	18.841	1.00	15.21	BTKA
ATOM	172	N	ALA	420	50.787	18.063	19.411	1.00	12.74	BTKA
ATOM	173	CA	ALA	420	51.152	17.747	18.034	1.00	10.26	BTKA
ATOM	174	CB	ALA	420	52.660	17.800	17.855	1.00	10.16	BTKA
ATOM	175	C	ALA	420	50.631	16.345	17.776	1.00	9.89	BTKA
ATOM	176	O	ALA	420	50.619	15.520	18.685	1.00	8.22	BTKA
ATOM	177	N	TRP	421	50.185	16.073	16.557	1.00	10.66	BTKA
ATOM	178	CA	TRP	421	49.637	14.759	16.236	1.00	14.79	BTKA
ATOM	179	CB	TRP	421	48.117	14.878	16.060	1.00	13.99	BTKA
ATOM	180	CG	TRP	421	47.433	13.605	15.683	1.00	15.77	BTKA
ATOM	181	CD2	TRP	421	46.685	13.355	14.486	1.00	17.12	BTKA
ATOM	182	CE2	TRP	421	46.203	12.027	14.563	1.00	19.95	BTKA
ATOM	183	CE3	TRP	421	46.373	14.123	13.357	1.00	13.78	BTKA
ATOM	184	CD1	TRP	421	47.380	12.452	16.414	1.00	18.99	BTKA
ATOM	185	NE1	TRP	421	46.646	11.498	15.746	1.00	21.46	BTKA
ATOM	186	CZ2	TRP	421	45.419	11.454	13.552	1.00	19.23	BTKA
ATOM	187	CZ3	TRP	421	45.595	13.552	12.354	1.00	9.53	BTKA
ATOM	188	CH2	TRP	421	45.127	12.233	12.460	1.00	12.55	BTKA
ATOM	189	C	TRP	421	50.270	14.085	15.011	1.00	16.84	BTKA
ATOM	190	O	TRP	421	50.448	14.721	13.969	1.00	17.90	BTKA
ATOM	191	N	ARG	422	50.600	12.799	15.158	1.00	18.95	BTKA
ATOM	192	CA	ARG	422	51.194	11.983	14.091	1.00	24.07	BTKA
ATOM	193	CB	ARG	422	50.111	11.437	13.144	1.00	24.28	BTKA
ATOM	194	CG	ARG	422	49.243	10.342	13.724	1.00	21.64	BTKA
ATOM	195	CD	ARG	422	48.551	9.548	12.621	1.00	22.23	BTKA
ATOM	196	NE	ARG	422	47.770	10.392	11.720	1.00	25.72	BTKA
ATOM	197	CZ	ARG	422	46.956	9.936	10.769	1.00	26.16	BTKA
ATOM	198	NH1	ARG	422	46.292	10.799	10.011	1.00	24.22	BTKA
ATOM	199	NH2	ARG	422	46.799	8.630	10.568	1.00	25.98	BTKA
ATOM	200	C	ARG	422	52.263	12.701	13.267	1.00	26.23	BTKA
ATOM	201	O	ARG	422	52.163	12.802	12.043	1.00	25.36	BTKA
ATOM	202	N	GLY	423	53.308	13.160	13.935	1.00	28.03	BTKA
ATOM	203	CA	GLY	423	54.347	13.876	13.234	1.00	28.68	BTKA
ATOM	204	C	GLY	423	54.117	15.347	13.502	1.00	31.49	BTKA
ATOM	205	O	GLY	423	54.093	15.758	14.666	1.00	33.41	BTKA
ATOM	206	N	ALA	424	53.831	16.124	12.460	1.00	30.81	BTKA
ATOM	207	CA	ALA	424	53.635	17.553	12.660	1.00	29.14	BTKA
ATOM	208	CB	ALA	424	54.793	18.322	12.067	1.00	32.15	BTKA
ATOM	209	C	ALA	424	52.301	18.185	12.256	1.00	25.28	BTKA
ATOM	210	O	ALA	424	52.227	18.989	11.324	1.00	22.96	BTKA
ATOM	211	N	ALA	425	51.249	17.822	12.978	1.00	21.73	BTKA
ATOM	212	CA	ALA	425	49.936	18.390	12.753	1.00	17.25	BTKA
ATOM	213	CB	ALA	425	48.910	17.300	12.468	1.00	14.79	BTKA
ATOM	214	C	ALA	425	49.623	19.102	14.062	1.00	17.01	BTKA
ATOM	215	O	ALA	425	49.656	18.490	15.128	1.00	16.50	BTKA
ATOM	216	N	ASP	426	49.445	20.415	13.996	1.00	16.77	BTKA
ATOM	217	CA	ASP	426	49.137	21.200	15.179	1.00	14.51	BTKA
ATOM	218	CB	ASP	426	49.418	22.681	14.926	1.00	16.45	BTKA
ATOM	219	CG	ASP	426	50.882	22.956	14.643	1.00	20.73	BTKA
ATOM	220	OD1	ASP	426	51.185	23.493	13.558	1.00	19.46	BTKA
ATOM	221	OD2	ASP	426	51.732	22.637	15.504	1.00	22.08	BTKA
ATOM	222	C	ASP	426	47.672	20.983	15.507	1.00	15.14	BTKA
ATOM	223	O	ASP	426	46.796	21.258	14.682	1.00	15.14	BTKA
ATOM	224	N	VAL	427	47.408	20.473	16.706	1.00	15.54	BTKA
ATOM	225	CA	VAL	427	46.046	20.196	17.125	1.00	12.56	BTKA
ATOM	226	CB	VAL	427	45.814	18.664	17.291	1.00	13.80	BTKA

Atom Number	Atom Type	Amino Acid Residue		X	Y	Z	Occ.	Temp Factor	
ATOM	227	CG1	VAL 427	46.243	17.926	16.041	1.00	7.25	BTKA
ATOM	228	CG2	VAL 427	46.557	18.122	18.511	1.00	13.29	BTKA
ATOM	229	C	VAL 427	45.659	20.908	18.421	1.00	12.59	BTKA
ATOM	230	O	VAL 427	46.516	21.391	19.166	1.00	15.43	BTKA
ATOM	231	N	ALA 428	44.354	21.023	18.634	1.00	11.11	BTKA
ATOM	232	CA	ALA 428	43.785	21.637	19.822	1.00	12.87	BTKA
ATOM	233	CB	ALA 428	42.995	22.872	19.449	1.00	9.07	BTKA
ATOM	234	C	ALA 428	42.860	20.565	20.380	1.00	12.26	BTKA
ATOM	235	O	ALA 428	41.833	20.263	19.775	1.00	17.33	BTKA
ATOM	236	N	ILE 429	43.246	19.957	21.501	1.00	16.62	BTKA
ATOM	237	CA	ILE 429	42.461	18.889	22.117	1.00	15.64	BTKA
ATOM	238	CB	ILE 429	43.383	17.773	22.733	1.00	14.98	BTKA
ATOM	239	CG2	ILE 429	44.844	18.223	22.770	1.00	13.61	BTKA
ATOM	240	CG1	ILE 429	42.855	17.290	24.088	1.00	15.92	BTKA
ATOM	241	CD	ILE 429	43.679	16.183	24.712	1.00	20.29	BTKA
ATOM	242	C	ILE 429	41.342	19.321	23.067	1.00	16.00	BTKA
ATOM	243	O	ILE 429	41.583	19.938	24.114	1.00	12.97	BTKA
ATOM	244	N	LYS 430	40.112	19.013	22.657	1.00	20.23	BTKA
ATOM	245	CA	LYS 430	38.892	19.327	23.403	1.00	22.33	BTKA
ATOM	246	CB	LYS 430	37.769	19.692	22.422	1.00	25.59	BTKA
ATOM	247	CG	LYS 430	36.474	20.199	23.049	1.00	29.20	BTKA
ATOM	248	CD	LYS 430	35.457	20.560	21.963	1.00	31.15	BTKA
ATOM	249	CE	LYS 430	34.196	21.193	22.544	1.00	32.32	BTKA
ATOM	250	NZ	LYS 430	33.185	21.522	21.491	1.00	25.96	BTKA
ATOM	251	C	LYS 430	38.454	18.119	24.208	1.00	21.53	BTKA
ATOM	252	O	LYS 430	38.614	16.984	23.767	1.00	23.61	BTKA
ATOM	253	N	MET 431	37.899	18.364	25.385	1.00	22.32	BTKA
ATOM	254	CA	MET 431	37.420	17.281	26.232	1.00	25.57	BTKA
ATOM	255	CB	MET 431	37.831	17.490	27.696	1.00	23.66	BTKA
ATOM	256	CG	MET 431	39.313	17.321	27.980	1.00	28.55	BTKA
ATOM	257	SD	MET 431	39.644	17.035	29.737	1.00	29.62	BTKA
ATOM	258	CE	MET 431	39.350	18.692	30.411	1.00	25.27	BTKA
ATOM	259	C	MET 431	35.906	17.271	26.143	1.00	24.67	BTKA
ATOM	260	O	MET 431	35.288	18.316	25.941	1.00	27.00	BTKA
ATOM	261	N	ILE 432	35.320	16.084	26.199	1.00	26.73	BTKA
ATOM	262	CA	ILE 432	33.871	15.969	26.178	1.00	30.90	BTKA
ATOM	263	CB	ILE 432	33.392	14.792	25.284	1.00	32.72	BTKA
ATOM	264	CG2	ILE 432	31.937	14.456	25.569	1.00	29.29	BTKA
ATOM	265	CG1	ILE 432	33.547	15.149	23.802	1.00	31.51	BTKA
ATOM	266	CD	ILE 432	34.977	15.269	23.324	1.00	30.77	BTKA
ATOM	267	C	ILE 432	33.450	15.767	27.638	1.00	32.06	BTKA
ATOM	268	O	ILE 432	32.315	16.075	28.011	1.00	33.24	BTKA
ATOM	269	N	LYS 433	34.419	15.307	28.440	1.00	33.53	BTKA
ATOM	270	CA	LYS 433	34.341	15.031	29.885	1.00	34.00	BTKA
ATOM	271	CB	LYS 433	33.097	15.629	30.549	1.00	31.21	BTKA
ATOM	272	CG	LYS 433	33.169	17.155	30.714	1.00	30.57	BTKA
ATOM	273	CD	LYS 433	33.736	17.553	32.070	1.00	25.39	BTKA
ATOM	274	CE	LYS 433	32.746	17.249	33.191	1.00	24.00	BTKA
ATOM	275	NZ	LYS 433	31.467	17.997	33.006	1.00	15.65	BTKA
ATOM	276	C	LYS 433	34.519	13.555	30.235	1.00	35.56	BTKA
ATOM	277	O	LYS 433	34.910	12.755	29.384	1.00	36.53	BTKA
ATOM	278	N	GLU 434	34.292	13.210	31.500	1.00	35.04	BTKA
ATOM	279	CA	GLU 434	34.464	11.841	31.979	1.00	31.68	BTKA
ATOM	280	CB	GLU 434	35.236	11.859	33.299	1.00	31.76	BTKA
ATOM	281	CG	GLU 434	35.525	10.480	33.868	1.00	25.49	BTKA
ATOM	282	CD	GLU 434	36.019	10.534	35.283	1.00	25.78	BTKA
ATOM	283	OE1	GLU 434	35.196	10.333	36.191	1.00	30.32	BTKA
ATOM	284	OE2	GLU 434	37.222	10.776	35.491	1.00	30.52	BTKA

Atom Number	Atom Type	Amino Acid Residue		X	Y	Z	Occ.	Temp Factor	
ATOM 285	C	GLU	434	33.159	11.074	32.177	1.00	31.82	BTKA
ATOM 286	O	GLU	434	32.313	11.481	32.969	1.00	28.09	BTKA
ATOM 287	N	GLY	435	33.031	9.938	31.495	1.00	34.12	BTKA
ATOM 288	CA	GLY	435	31.844	9.110	31.610	1.00	35.84	BTKA
ATOM 289	C	GLY	435	30.583	9.721	31.023	1.00	37.43	BTKA
ATOM 290	O	GLY	435	29.953	9.120	30.144	1.00	36.18	BTKA
ATOM 291	N	SER	436	30.200	10.880	31.562	1.00	37.72	BTKA
ATOM 292	CA	SER	436	29.024	11.656	31.157	1.00	35.78	BTKA
ATOM 293	CB	SER	436	29.380	13.149	31.108	1.00	35.22	BTKA
ATOM 294	OG	SER	436	30.577	13.383	30.374	1.00	28.66	BTKA
ATOM 295	C	SER	436	28.442	11.227	29.825	1.00	34.88	BTKA
ATOM 296	O	SER	436	27.311	10.745	29.752	1.00	33.75	BTKA
ATOM 297	N	MET	437	29.236	11.407	28.778	1.00	35.33	BTKA
ATOM 298	CA	MET	437	28.848	11.037	27.432	1.00	36.32	BTKA
ATOM 299	CB	MET	437	29.146	12.191	26.467	1.00	35.52	BTKA
ATOM 300	CG	MET	437	28.879	13.578	27.063	1.00	36.44	BTKA
ATOM 301	SD	MET	437	27.262	13.773	27.876	1.00	30.54	BTKA
ATOM 302	CE	MET	437	26.468	14.965	26.768	1.00	30.24	BTKA
ATOM 303	C	MET	437	29.702	9.815	27.112	1.00	35.84	BTKA
ATOM 304	O	MET	437	30.916	9.829	27.323	1.00	33.00	BTKA
ATOM 305	N	SER	438	29.060	8.741	26.668	1.00	38.82	BTKA
ATOM 306	CA	SER	438	29.770	7.507	26.353	1.00	39.46	BTKA
ATOM 307	CB	SER	438	28.923	6.288	26.739	1.00	39.31	BTKA
ATOM 308	OG	SER	438	28.946	6.080	28.141	1.00	42.46	BTKA
ATOM 309	C	SER	438	30.291	7.349	24.928	1.00	37.92	BTKA
ATOM 310	O	SER	438	29.699	7.844	23.964	1.00	35.58	BTKA
ATOM 311	N	GLU	439	31.387	6.598	24.830	1.00	38.56	BTKA
ATOM 312	CA	GLU	439	32.072	6.281	23.579	1.00	37.22	BTKA
ATOM 313	CB	GLU	439	33.015	5.098	23.820	1.00	38.03	BTKA
ATOM 314	CG	GLU	439	33.578	4.444	22.567	1.00	39.09	BTKA
ATOM 315	CD	GLU	439	34.595	3.357	22.887	1.00	36.27	BTKA
ATOM 316	OE1	GLU	439	34.313	2.514	23.771	1.00	36.28	BTKA
ATOM 317	OE2	GLU	439	35.677	3.350	22.257	1.00	32.61	BTKA
ATOM 318	C	GLU	439	31.122	5.968	22.428	1.00	36.18	BTKA
ATOM 319	O	GLU	439	31.254	6.535	21.347	1.00	37.11	BTKA
ATOM 320	N	ASP	440	30.154	5.090	22.678	1.00	35.64	BTKA
ATOM 321	CA	ASP	440	29.172	4.692	21.665	1.00	36.29	BTKA
ATOM 322	CB	ASP	440	28.228	3.619	22.223	1.00	35.13	BTKA
ATOM 323	CG	ASP	440	28.822	2.223	22.157	1.00	33.91	BTKA
ATOM 324	OD1	ASP	440	29.754	1.921	22.933	1.00	33.93	BTKA
ATOM 325	OD2	ASP	440	28.342	1.425	21.328	1.00	33.14	BTKA
ATOM 326	C	ASP	440	28.343	5.838	21.089	1.00	35.32	BTKA
ATOM 327	O	ASP	440	28.079	5.876	19.884	1.00	31.62	BTKA
ATOM 328	N	GLU	441	27.939	6.764	21.954	1.00	34.63	BTKA
ATOM 329	CA	GLU	441	27.120	7.905	21.546	1.00	33.66	BTKA
ATOM 330	CB	GLU	441	26.845	8.819	22.742	1.00	35.94	BTKA
ATOM 331	CG	GLU	441	26.422	8.150	24.039	1.00	35.11	BTKA
ATOM 332	CD	GLU	441	26.394	9.138	25.203	1.00	35.16	BTKA
ATOM 333	OE1	GLU	441	26.838	10.292	25.024	1.00	36.46	BTKA
ATOM 334	OE2	GLU	441	25.946	8.765	26.306	1.00	35.56	BTKA
ATOM 335	C	GLU	441	27.786	8.756	20.462	1.00	32.20	BTKA
ATOM 336	O	GLU	441	27.301	8.861	19.333	1.00	29.93	BTKA
ATOM 337	N	PHE	442	28.908	9.361	20.841	1.00	31.11	BTKA
ATOM 338	CA	PHE	442	29.683	10.253	19.987	1.00	29.28	BTKA
ATOM 339	CB	PHE	442	30.854	10.837	20.804	1.00	29.09	BTKA
ATOM 340	CG	PHE	442	31.563	11.990	20.135	1.00	31.98	BTKA
ATOM 341	CD1	PHE	442	30.865	12.888	19.325	1.00	32.20	BTKA
ATOM 342	CD2	PHE	442	32.932	12.173	20.308	1.00	30.79	BTKA

	Atom Number	Atom Type	Amino Acid Residue		X	Y	Z	Occ.	Temp Factor	
ATOM	343	CE1	PHE	442	31.517	13.947	18.697	1.00	27.29	BTKA
ATOM	344	CE2	PHE	442	33.592	13.229	19.684	1.00	29.97	BTKA
ATOM	345	CZ	PHE	442	32.879	14.117	18.876	1.00	27.41	BTKA
ATOM	346	C	PHE	442	30.182	9.638	18.671	1.00	27.25	BTKA
ATOM	347	O	PHE	442	30.363	10.351	17.688	1.00	26.62	BTKA
ATOM	348	N	ILE	443	30.377	8.325	18.646	1.00	26.46	BTKA
ATOM	349	CA	ILE	443	30.866	7.639	17.450	1.00	26.92	BTKA
ATOM	350	CB	ILE	443	30.753	6.097	17.608	1.00	27.02	BTKA
ATOM	351	CG2	ILE	443	30.893	5.399	16.262	1.00	29.28	BTKA
ATOM	352	CG1	ILE	443	31.808	5.586	18.602	1.00	26.98	BTKA
ATOM	353	CD	ILE	443	33.253	5.879	18.207	1.00	23.34	BTKA
ATOM	354	C	ILE	443	30.173	8.079	16.160	1.00	27.64	BTKA
ATOM	355	O	ILE	443	30.834	8.451	15.189	1.00	27.13	BTKA
ATOM	356	N	GLU	444	28.843	8.057	16.163	1.00	29.25	BTKA
ATOM	357	CA	GLU	444	28.061	8.449	14.992	1.00	30.51	BTKA
ATOM	358	CB	GLU	444	26.552	8.274	15.256	1.00	32.35	BTKA
ATOM	359	CG	GLU	444	26.053	8.917	16.553	1.00	35.88	BTKA
ATOM	360	CD	GLU	444	24.549	9.144	16.582	1.00	35.26	BTKA
ATOM	361	OE1	GLU	444	24.116	10.292	16.319	1.00	33.49	BTKA
ATOM	362	OE2	GLU	444	23.802	8.186	16.886	1.00	36.30	BTKA
ATOM	363	C	GLU	444	28.353	9.886	14.571	1.00	29.10	BTKA
ATOM	364	O	GLU	444	28.781	10.139	13.445	1.00	29.32	BTKA
ATOM	365	N	GLU	445	28.173	10.816	15.502	1.00	26.25	BTKA
ATOM	366	CA	GLU	445	28.384	12.226	15.229	1.00	25.93	BTKA
ATOM	367	CB	GLU	445	27.935	13.073	16.420	1.00	24.15	BTKA
ATOM	368	CG	GLU	445	26.435	12.964	16.694	1.00	25.82	BTKA
ATOM	369	CD	GLU	445	25.860	14.206	17.357	1.00	26.92	BTKA
ATOM	370	OE1	GLU	445	25.282	14.077	18.454	1.00	21.98	BTKA
ATOM	371	OE2	GLU	445	25.973	15.308	16.775	1.00	27.91	BTKA
ATOM	372	C	GLU	445	29.817	12.534	14.835	1.00	26.08	BTKA
ATOM	373	O	GLU	445	30.075	13.505	14.117	1.00	26.43	BTKA
ATOM	374	N	ALA	446	30.739	11.679	15.272	1.00	26.04	BTKA
ATOM	375	CA	ALA	446	32.152	11.831	14.949	1.00	24.80	BTKA
ATOM	376	CB	ALA	446	32.998	10.909	15.813	1.00	24.38	BTKA
ATOM	377	C	ALA	446	32.346	11.504	13.468	1.00	24.74	BTKA
ATOM	378	O	ALA	446	33.003	12.264	12.746	1.00	23.97	BTKA
ATOM	379	N	LYS	447	31.755	10.391	13.020	1.00	22.24	BTKA
ATOM	380	CA	LYS	447	31.841	9.971	11.620	1.00	20.97	BTKA
ATOM	381	CB	LYS	447	31.065	8.669	11.380	1.00	20.58	BTKA
ATOM	382	CG	LYS	447	31.559	7.450	12.143	1.00	22.18	BTKA
ATOM	383	CD	LYS	447	30.767	6.201	11.752	1.00	22.45	BTKA
ATOM	384	CE	LYS	447	30.957	5.063	12.752	1.00	23.27	BTKA
ATOM	385	NZ	LYS	447	32.367	4.595	12.843	1.00	25.50	BTKA
ATOM	386	C	LYS	447	31.223	11.066	10.762	1.00	20.28	BTKA
ATOM	387	O	LYS	447	31.770	11.457	9.727	1.00	18.27	BTKA
ATOM	388	N	VAL	448	30.068	11.544	11.210	1.00	22.03	BTKA
ATOM	389	CA	VAL	448	29.332	12.599	10.532	1.00	23.98	BTKA
ATOM	390	CB	VAL	448	27.996	12.881	11.266	1.00	26.86	BTKA
ATOM	391	CG1	VAL	448	27.403	14.218	10.835	1.00	26.50	BTKA
ATOM	392	CG2	VAL	448	27.013	11.760	10.976	1.00	24.51	BTKA
ATOM	393	C	VAL	448	30.154	13.886	10.382	1.00	23.84	BTKA
ATOM	394	O	VAL	448	30.177	14.479	9.304	1.00	22.58	BTKA
ATOM	395	N	MET	449	30.848	14.300	11.439	1.00	25.01	BTKA
ATOM	396	CA	MET	449	31.659	15.514	11.375	1.00	26.00	BTKA
ATOM	397	CB	MET	449	32.036	15.992	12.775	1.00	28.34	BTKA
ATOM	398	CG	MET	449	30.941	16.778	13.471	1.00	29.82	BTKA
ATOM	399	SD	MET	449	31.446	17.269	15.116	1.00	32.37	BTKA
ATOM	400	CE	MET	449	32.786	18.412	14.721	1.00	32.43	BTKA

	Atom Number	Atom Type	Amino Acid Residue		X	Y	Z	Occ.	Temp Factor	
ATOM	401	C	MET	449	32.910	15.374	10.514	1.00	26.88	BTKA
ATOM	402	O	MET	449	33.239	16.271	9.742	1.00	24.06	BTKA
ATOM	403	N	MET	450	33.610	14.254	10.645	1.00	29.26	BTKA
ATOM	404	CA	MET	450	34.811	14.023	9.849	1.00	31.06	BTKA
ATOM	405	CB	MET	450	35.558	12.780	10.336	1.00	34.52	BTKA
ATOM	406	CG	MET	450	36.186	12.976	11.709	1.00	35.20	BTKA
ATOM	407	SD	MET	450	37.355	11.695	12.173	1.00	38.54	BTKA
ATOM	408	CE	MET	450	36.287	10.551	13.085	1.00	33.93	BTKA
ATOM	409	C	MET	450	34.502	13.938	8.351	1.00	28.32	BTKA
ATOM	410	O	MET	450	35.390	14.091	7.517	1.00	27.65	BTKA
ATOM	411	N	ASN	451	33.244	13.680	8.007	1.00	27.43	BTKA
ATOM	412	CA	ASN	451	32.853	13.636	6.603	1.00	25.78	BTKA
ATOM	413	CB	ASN	451	31.515	12.912	6.417	1.00	25.17	BTKA
ATOM	414	CG	ASN	451	31.681	11.499	5.858	1.00	24.38	BTKA
ATOM	415	OD1	ASN	451	30.703	10.778	5.673	1.00	24.24	BTKA
ATOM	416	ND2	ASN	451	32.919	11.104	5.576	1.00	27.13	BTKA
ATOM	417	C	ASN	451	32.781	15.071	6.073	1.00	24.17	BTKA
ATOM	418	O	ASN	451	32.831	15.308	4.862	1.00	23.10	BTKA
ATOM	419	N	LEU	452	32.656	16.025	6.989	1.00	23.71	BTKA
ATOM	420	CA	LEU	452	32.616	17.436	6.627	1.00	21.99	BTKA
ATOM	421	CB	LEU	452	32.023	18.279	7.767	1.00	18.83	BTKA
ATOM	422	CG	LEU	452	30.602	18.795	7.552	1.00	14.55	BTKA
ATOM	423	CD1	LEU	452	29.724	17.669	7.063	1.00	13.88	BTKA
ATOM	424	CD2	LEU	452	30.064	19.402	8.828	1.00	16.37	BTKA
ATOM	425	C	LEU	452	34.055	17.854	6.387	1.00	22.15	BTKA
ATOM	426	O	LEU	452	34.966	17.356	7.041	1.00	26.28	BTKA
ATOM	427	N	SER	453	34.267	18.720	5.414	1.00	18.69	BTKA
ATOM	428	CA	SER	453	35.598	19.194	5.117	1.00	17.44	BTKA
ATOM	429	CB	SER	453	36.468	18.074	4.552	1.00	20.39	BTKA
ATOM	430	OG	SER	453	37.270	17.498	5.569	1.00	32.76	BTKA
ATOM	431	C	SER	453	35.551	20.344	4.147	1.00	15.35	BTKA
ATOM	432	O	SER	453	34.960	20.253	3.083	1.00	16.35	BTKA
ATOM	433	N	HIS	454	36.153	21.445	4.554	1.00	11.81	BTKA
ATOM	434	CA	HIS	454	36.240	22.647	3.753	1.00	9.84	BTKA
ATOM	435	CB	HIS	454	34.942	23.469	3.833	1.00	11.56	BTKA
ATOM	436	CG	HIS	454	34.869	24.572	2.821	1.00	5.59	BTKA
ATOM	437	CD2	HIS	454	34.345	24.601	1.574	1.00	3.51	BTKA
ATOM	438	ND1	HIS	454	35.448	25.806	3.020	1.00	2.00	BTKA
ATOM	439	CE1	HIS	454	35.292	26.545	1.935	1.00	3.01	BTKA
ATOM	440	NE2	HIS	454	34.625	25.837	1.044	1.00	4.91	BTKA
ATOM	441	C	HIS	454	37.361	23.382	4.449	1.00	9.19	BTKA
ATOM	442	O	HIS	454	37.456	23.331	5.676	1.00	8.32	BTKA
ATOM	443	N	GLU	455	38.232	24.028	3.682	1.00	10.17	BTKA
ATOM	444	CA	GLU	455	39.351	24.770	4.262	1.00	10.17	BTKA
ATOM	445	CB	GLU	455	40.280	25.267	3.154	1.00	13.02	BTKA
ATOM	446	CG	GLU	455	39.603	26.176	2.162	1.00	15.79	BTKA
ATOM	447	CD	GLU	455	40.544	26.677	1.091	1.00	20.82	BTKA
ATOM	448	OE1	GLU	455	40.670	27.909	0.940	1.00	24.47	BTKA
ATOM	449	OE2	GLU	455	41.145	25.840	0.387	1.00	24.08	BTKA
ATOM	450	C	GLU	455	38.913	25.952	5.141	1.00	12.87	BTKA
ATOM	451	O	GLU	455	39.748	26.617	5.762	1.00	14.07	BTKA
ATOM	452	N	LYS	456	37.611	26.234	5.163	1.00	8.19	BTKA
ATOM	453	CA	LYS	456	37.084	27.334	5.963	1.00	7.61	BTKA
ATOM	454	CB	LYS	456	36.272	28.282	5.078	1.00	6.39	BTKA
ATOM	455	CG	LYS	456	37.102	28.927	3.974	1.00	9.24	BTKA
ATOM	456	CD	LYS	456	38.167	29.879	4.537	1.00	11.93	BTKA
ATOM	457	CE	LYS	456	39.236	30.217	3.493	1.00	13.97	BTKA
ATOM	458	NZ	LYS	456	38.693	30.793	2.222	1.00	11.85	BTKA

	Atom Number	Atom Type	Amino Acid Residue		X	Y	Z	Occ.	Temp Factor	
ATOM	459	C	LYS	456	36.266	26.821	7.152	1.00	5.26	BTKA
ATOM	460	O	LYS	456	35.500	27.555	7.770	1.00	3.31	BTKA
ATOM	461	N	LEU	457	36.419	25.533	7.429	1.00	7.43	BTKA
ATOM	462	CA	LEU	457	35.747	24.870	8.542	1.00	7.04	BTKA
ATOM	463	CB	LEU	457	34.833	23.732	8.051	1.00	5.48	BTKA
ATOM	464	CG	LEU	457	33.423	24.015	7.512	1.00	12.38	BTKA
ATOM	465	CD1	LEU	457	32.887	22.821	6.734	1.00	6.71	BTKA
ATOM	466	CD2	LEU	457	32.491	24.355	8.648	1.00	2.00	BTKA
ATOM	467	C	LEU	457	36.886	24.267	9.335	1.00	5.80	BTKA
ATOM	468	O	LEU	457	37.797	23.684	8.756	1.00	8.77	BTKA
ATOM	469	N	VAL	458	36.897	24.497	10.638	1.00	5.47	BTKA
ATOM	470	CA	VAL	458	37.928	23.925	11.478	1.00	5.34	BTKA
ATOM	471	CB	VAL	458	37.817	24.471	12.907	1.00	5.74	BTKA
ATOM	472	CG1	VAL	458	38.738	23.703	13.862	1.00	4.86	BTKA
ATOM	473	CG2	VAL	458	38.169	25.956	12.901	1.00	2.00	BTKA
ATOM	474	C	VAL	458	37.645	22.427	11.404	1.00	9.05	BTKA
ATOM	475	O	VAL	458	36.517	21.990	11.660	1.00	8.51	BTKA
ATOM	476	N	GLN	459	38.640	21.670	10.947	1.00	12.50	BTKA
ATOM	477	CA	GLN	459	38.532	20.223	10.769	1.00	11.11	BTKA
ATOM	478	CB	GLN	459	39.567	19.716	9.751	1.00	12.18	BTKA
ATOM	479	CG	GLN	459	39.885	20.639	8.588	1.00	14.96	BTKA
ATOM	480	CD	GLN	459	38.883	20.575	7.462	1.00	16.30	BTKA
ATOM	481	OE1	GLN	459	37.686	20.837	7.644	1.00	18.40	BTKA
ATOM	482	NE2	GLN	459	39.375	20.255	6.265	1.00	15.08	BTKA
ATOM	483	C	GLN	459	38.737	19.413	12.034	1.00	10.27	BTKA
ATOM	484	O	GLN	459	39.607	19.710	12.855	1.00	10.07	BTKA
ATOM	485	N	LEU	460	37.964	18.345	12.143	1.00	11.55	BTKA
ATOM	486	CA	LEU	460	38.069	17.422	13.253	1.00	12.61	BTKA
ATOM	487	CB	LEU	460	36.702	16.791	13.552	1.00	10.46	BTKA
ATOM	488	CG	LEU	460	36.480	16.009	14.854	1.00	9.21	BTKA
ATOM	489	CD1	LEU	460	35.616	14.793	14.552	1.00	10.03	BTKA
ATOM	490	CD2	LEU	460	37.789	15.552	15.490	1.00	10.95	BTKA
ATOM	491	C	LEU	460	39.012	16.356	12.712	1.00	12.22	BTKA
ATOM	492	O	LEU	460	38.832	15.883	11.588	1.00	9.11	BTKA
ATOM	493	N	TYR	461	40.019	15.988	13.496	1.00	14.03	BTKA
ATOM	494	CA	TYR	461	40.970	14.972	13.063	1.00	17.98	BTKA
ATOM	495	CB	TYR	461	42.385	15.311	13.531	1.00	15.90	BTKA
ATOM	496	CG	TYR	461	42.994	16.477	12.797	1.00	14.99	BTKA
ATOM	497	CD1	TYR	461	43.523	17.553	13.489	1.00	10.88	BTKA
ATOM	498	CE1	TYR	461	44.047	18.645	12.821	1.00	18.55	BTKA
ATOM	499	CD2	TYR	461	43.007	16.517	11.403	1.00	18.59	BTKA
ATOM	500	CE2	TYR	461	43.532	17.611	10.720	1.00	18.77	BTKA
ATOM	501	CZ	TYR	461	44.046	18.673	11.439	1.00	18.48	BTKA
ATOM	502	OH	TYR	461	44.539	19.774	10.780	1.00	17.96	BTKA
ATOM	503	C	TYR	461	40.593	13.578	13.527	1.00	19.94	BTKA
ATOM	504	O	TYR	461	40.611	12.630	12.747	1.00	20.11	BTKA
ATOM	505	N	GLY	462	40.226	13.455	14.796	1.00	22.97	BTKA
ATOM	506	CA	GLY	462	39.872	12.155	15.319	1.00	21.20	BTKA
ATOM	507	C	GLY	462	39.280	12.224	16.705	1.00	19.72	BTKA
ATOM	508	O	GLY	462	39.205	13.291	17.320	1.00	15.82	BTKA
ATOM	509	N	VAL	463	38.841	11.070	17.186	1.00	17.64	BTKA
ATOM	510	CA	VAL	463	38.231	10.961	18.494	1.00	19.56	BTKA
ATOM	511	CB	VAL	463	36.778	10.448	18.397	1.00	14.65	BTKA
ATOM	512	CG1	VAL	463	35.920	11.446	17.649	1.00	12.04	BTKA
ATOM	513	CG2	VAL	463	36.737	9.090	17.715	1.00	16.09	BTKA
ATOM	514	C	VAL	463	39.036	10.004	19.345	1.00	22.19	BTKA
ATOM	515	O	VAL	463	39.563	9.008	18.851	1.00	26.83	BTKA
ATOM	516	N	CYS	464	39.170	10.340	20.617	1.00	26.12	BTKA

Atom Number	Atom Type	Amino Acid Residue		X	Y	Z	Occ.	Temp Factor	
ATOM	517	CA	CYS 464	39.893	9.505	21.559	1.00	28.36	BTKA
ATOM	518	CB	CYS 464	41.077	10.279	22.153	1.00	28.93	BTKA
ATOM	519	SG	CYS 464	42.375	9.282	22.957	1.00	33.22	BTKA
ATOM	520	C	CYS 464	38.834	9.182	22.613	1.00	31.37	BTKA
ATOM	521	O	CYS 464	38.850	9.707	23.726	1.00	32.82	BTKA
ATOM	522	N	THR 465	37.859	8.377	22.204	1.00	32.79	BTKA
ATOM	523	CA	THR 465	36.759	7.968	23.071	1.00	33.01	BTKA
ATOM	524	CB	THR 465	35.521	7.569	22.227	1.00	31.07	BTKA
ATOM	525	OG1	THR 465	35.870	6.490	21.350	1.00	30.45	BTKA
ATOM	526	CG2	THR 465	35.026	8.741	21.397	1.00	28.93	BTKA
ATOM	527	C	THR 465	37.150	6.759	23.921	1.00	34.05	BTKA
ATOM	528	O	THR 465	36.283	6.010	24.378	1.00	31.83	BTKA
ATOM	529	N	LYS 466	38.447	6.571	24.138	1.00	35.70	BTKA
ATOM	530	CA	LYS 466	38.926	5.426	24.901	1.00	36.53	BTKA
ATOM	531	CB	LYS 466	40.447	5.308	24.793	1.00	35.48	BTKA
ATOM	532	CG	LYS 466	40.955	4.991	23.376	1.00	38.68	BTKA
ATOM	533	CD	LYS 466	40.542	3.589	22.894	1.00	39.29	BTKA
ATOM	534	CE	LYS 466	39.081	3.514	22.451	1.00	38.59	BTKA
ATOM	535	NZ	LYS 466	38.664	2.137	22.077	1.00	40.01	BTKA
ATOM	536	C	LYS 466	38.461	5.332	26.349	1.00	36.75	BTKA
ATOM	537	O	LYS 466	39.215	5.624	27.278	1.00	34.39	BTKA
ATOM	538	N	GLN 467	37.226	4.861	26.513	1.00	37.31	BTKA
ATOM	539	CA	GLN 467	36.588	4.671	27.809	1.00	38.68	BTKA
ATOM	540	CB	GLN 467	37.121	3.402	28.476	1.00	36.64	BTKA
ATOM	541	CG	GLN 467	36.249	2.166	28.246	1.00	35.25	BTKA
ATOM	542	CD	GLN 467	35.842	1.967	26.787	1.00	33.56	BTKA
ATOM	543	OE1	GLN 467	36.529	2.412	25.864	1.00	32.22	BTKA
ATOM	544	NE2	GLN 467	34.716	1.289	26.578	1.00	27.03	BTKA
ATOM	545	C	GLN 467	36.671	5.870	28.743	1.00	40.26	BTKA
ATOM	546	O	GLN 467	35.659	6.531	29.004	1.00	43.24	BTKA
ATOM	547	N	ARG 468	37.860	6.118	29.282	1.00	40.19	BTKA
ATOM	548	CA	ARG 468	38.082	7.248	30.173	1.00	38.09	BTKA
ATOM	549	CB	ARG 468	39.501	7.183	30.746	1.00	35.92	BTKA
ATOM	550	CG	ARG 468	39.801	5.921	31.551	1.00	30.86	BTKA
ATOM	551	CD	ARG 468	38.832	5.707	32.719	1.00	32.42	BTKA
ATOM	552	NE	ARG 468	37.508	5.243	32.293	1.00	33.04	BTKA
ATOM	553	CZ	ARG 468	37.243	4.020	31.837	1.00	35.40	BTKA
ATOM	554	NH1	ARG 468	38.206	3.109	31.740	1.00	37.18	BTKA
ATOM	555	NH2	ARG 468	36.010	3.707	31.465	1.00	35.12	BTKA
ATOM	556	C	ARG 468	37.861	8.506	29.328	1.00	37.39	BTKA
ATOM	557	O	ARG 468	37.805	8.408	28.105	1.00	37.02	BTKA
ATOM	558	N	PRO 469	37.755	9.695	29.961	1.00	37.24	BTKA
ATOM	559	CD	PRO 469	38.219	9.958	31.336	1.00	35.17	BTKA
ATOM	560	CA	PRO 469	37.532	10.971	29.266	1.00	36.80	BTKA
ATOM	561	CB	PRO 469	38.542	11.886	29.943	1.00	36.83	BTKA
ATOM	562	CG	PRO 469	38.390	11.487	31.363	1.00	35.94	BTKA
ATOM	563	C	PRO 469	37.672	10.973	27.742	1.00	34.06	BTKA
ATOM	564	O	PRO 469	38.733	10.653	27.196	1.00	32.99	BTKA
ATOM	565	N	ILE 470	36.569	11.286	27.066	1.00	33.42	BTKA
ATOM	566	CA	ILE 470	36.537	11.338	25.608	1.00	29.80	BTKA
ATOM	567	CB	ILE 470	35.096	11.277	25.068	1.00	28.92	BTKA
ATOM	568	CG2	ILE 470	35.095	11.469	23.561	1.00	28.43	BTKA
ATOM	569	CG1	ILE 470	34.434	9.950	25.447	1.00	32.53	BTKA
ATOM	570	CD	ILE 470	32.980	9.858	25.017	1.00	31.41	BTKA
ATOM	571	C	ILE 470	37.156	12.645	25.148	1.00	28.29	BTKA
ATOM	572	O	ILE 470	36.724	13.725	25.563	1.00	28.16	BTKA
ATOM	573	N	PHE 471	38.171	12.542	24.302	1.00	26.48	BTKA
ATOM	574	CA	PHE 471	38.848	13.718	23.782	1.00	23.24	BTKA

	Atom Number	Atom Type	Amino Acid Residue		X	Y	Z	Occ.	Temp Factor	
ATOM	575	CB	PHE	471	40.362	13.623	24.005	1.00	26.91	BTKA
ATOM	576	CG	PHE	471	40.753	12.964	25.294	1.00	33.25	BTKA
ATOM	577	CD1	PHE	471	40.457	13.560	26.517	1.00	34.40	BTKA
ATOM	578	CD2	PHE	471	41.419	11.742	25.286	1.00	33.15	BTKA
ATOM	579	CE1	PHE	471	40.821	12.949	27.708	1.00	37.94	BTKA
ATOM	580	CE2	PHE	471	41.787	11.120	26.474	1.00	37.98	BTKA
ATOM	581	CZ	PHE	471	41.489	11.723	27.687	1.00	38.55	BTKA
ATOM	582	C	PHE	471	38.589	13.837	22.289	1.00	19.98	BTKA
ATOM	583	O	PHE	471	38.237	12.862	21.614	1.00	18.06	BTKA
ATOM	584	N	ILE	472	38.796	15.038	21.776	1.00	15.89	BTKA
ATOM	585	CA	ILE	472	38.624	15.310	20.367	1.00	16.13	BTKA
ATOM	586	CB	ILE	472	37.214	15.928	20.068	1.00	19.20	BTKA
ATOM	587	CG2	ILE	472	37.237	17.445	20.155	1.00	21.36	BTKA
ATOM	588	CG1	ILE	472	36.746	15.519	18.672	1.00	22.75	BTKA
ATOM	589	CD	ILE	472	35.491	16.217	18.204	1.00	19.43	BTKA
ATOM	590	C	ILE	472	39.763	16.270	20.030	1.00	15.65	BTKA
ATOM	591	O	ILE	472	40.164	17.076	20.876	1.00	14.58	BTKA
ATOM	592	N	ILE	473	40.374	16.081	18.861	1.00	12.55	BTKA
ATOM	593	CA	ILE	473	41.460	16.941	18.410	1.00	8.29	BTKA
ATOM	594	CB	ILE	473	42.760	16.179	18.121	1.00	6.11	BTKA
ATOM	595	CG2	ILE	473	43.512	15.930	19.394	1.00	8.19	BTKA
ATOM	596	CG1	ILE	473	42.469	14.896	17.351	1.00	12.26	BTKA
ATOM	597	CD	ILE	473	43.722	14.129	16.949	1.00	12.28	BTKA
ATOM	598	C	ILE	473	41.023	17.624	17.140	1.00	10.43	BTKA
ATOM	599	O	ILE	473	40.655	16.974	16.163	1.00	10.61	BTKA
ATOM	600	N	THR	474	41.039	18.943	17.169	1.00	10.11	BTKA
ATOM	601	CA	THR	474	40.646	19.740	16.031	1.00	12.13	BTKA
ATOM	602	CB	THR	474	39.527	20.724	16.452	1.00	13.64	BTKA
ATOM	603	OG1	THR	474	39.496	20.831	17.885	1.00	11.89	BTKA
ATOM	604	CG2	THR	474	38.169	20.231	15.967	1.00	14.36	BTKA
ATOM	605	C	THR	474	41.897	20.487	15.586	1.00	12.41	BTKA
ATOM	606	O	THR	474	42.914	20.444	16.278	1.00	12.99	BTKA
ATOM	607	N	GLU	475	41.862	21.114	14.413	1.00	14.37	BTKA
ATOM	608	CA	GLU	475	43.032	21.851	13.951	1.00	14.93	BTKA
ATOM	609	CB	GLU	475	42.927	22.210	12.462	1.00	14.14	BTKA
ATOM	610	CG	GLU	475	41.841	23.163	12.075	1.00	18.34	BTKA
ATOM	611	CD	GLU	475	41.887	23.516	10.590	1.00	18.18	BTKA
ATOM	612	OE1	GLU	475	42.827	24.212	10.143	1.00	19.64	BTKA
ATOM	613	OE2	GLU	475	40.976	23.102	9.860	1.00	17.68	BTKA
ATOM	614	C	GLU	475	43.267	23.084	14.813	1.00	15.03	BTKA
ATOM	615	O	GLU	475	42.311	23.751	15.216	1.00	16.87	BTKA
ATOM	616	N	TYR	476	44.533	23.327	15.156	1.00	16.03	BTKA
ATOM	617	CA	TYR	476	44.938	24.462	15.985	1.00	12.78	BTKA
ATOM	618	CB	TYR	476	46.367	24.263	16.516	1.00	14.76	BTKA
ATOM	619	CG	TYR	476	46.849	25.389	17.397	1.00	17.47	BTKA
ATOM	620	CD1	TYR	476	46.426	25.491	18.719	1.00	21.65	BTKA
ATOM	621	CE1	TYR	476	46.806	26.566	19.519	1.00	18.11	BTKA
ATOM	622	CD2	TYR	476	47.676	26.394	16.895	1.00	16.67	BTKA
ATOM	623	CE2	TYR	476	48.059	27.477	17.690	1.00	15.07	BTKA
ATOM	624	CZ	TYR	476	47.617	27.555	19.000	1.00	20.25	BTKA
ATOM	625	OH	TYR	476	47.963	28.621	19.801	1.00	22.07	BTKA
ATOM	626	C	TYR	476	44.864	25.760	15.202	1.00	9.86	BTKA
ATOM	627	O	TYR	476	45.291	25.822	14.053	1.00	12.02	BTKA
ATOM	628	N	MET	477	44.341	26.798	15.850	1.00	12.43	BTKA
ATOM	629	CA	MET	477	44.180	28.122	15.248	1.00	10.82	BTKA
ATOM	630	CB	MET	477	42.690	28.470	15.173	1.00	13.68	BTKA
ATOM	631	CG	MET	477	41.854	27.466	14.373	1.00	12.55	BTKA
ATOM	632	SD	MET	477	42.224	27.500	12.622	1.00	8.47	BTKA

Atom Number	Atom Type	Amino Acid Residue		X	Y	Z	Occ.	Temp Factor	
ATOM	633	CE	MET 477	41.240	28.862	12.158	1.00	8.85	BTKA
ATOM	634	C	MET 477	44.923	29.171	16.076	1.00	8.89	BTKA
ATOM	635	O	MET 477	44.402	29.665	17.076	1.00	10.46	BTKA
ATOM	636	N	ALA 478	46.112	29.547	15.613	1.00	8.05	BTKA
ATOM	637	CA	ALA 478	46.980	30.503	16.300	1.00	6.04	BTKA
ATOM	638	CB	ALA 478	48.218	30.762	15.478	1.00	6.02	BTKA
ATOM	639	C	ALA 478	46.437	31.822	16.827	1.00	7.42	BTKA
ATOM	640	O	ALA 478	46.895	32.297	17.862	1.00	9.51	BTKA
ATOM	641	N	ASN 479	45.508	32.452	16.127	1.00	8.70	BTKA
ATOM	642	CA	ASN 479	44.997	33.721	16.625	1.00	11.12	BTKA
ATOM	643	CB	ASN 479	44.736	34.705	15.482	1.00	10.56	BTKA
ATOM	644	CG	ASN 479	46.014	35.189	14.823	1.00	10.54	BTKA
ATOM	645	OD1	ASN 479	46.162	35.116	13.607	1.00	14.22	BTKA
ATOM	646	ND2	ASN 479	46.944	35.693	15.623	1.00	5.93	BTKA
ATOM	647	C	ASN 479	43.778	33.594	17.527	1.00	10.80	BTKA
ATOM	648	O	ASN 479	43.300	34.593	18.066	1.00	13.56	BTKA
ATOM	649	N	GLY 480	43.309	32.371	17.742	1.00	13.64	BTKA
ATOM	650	CA	GLY 480	42.153	32.165	18.600	1.00	18.12	BTKA
ATOM	651	C	GLY 480	40.822	32.436	17.919	1.00	18.79	BTKA
ATOM	652	O	GLY 480	40.670	32.194	16.723	1.00	18.15	BTKA
ATOM	653	N	CYS 481	39.844	32.921	18.679	1.00	20.27	BTKA
ATOM	654	CA	CYS 481	38.534	33.210	18.108	1.00	16.03	BTKA
ATOM	655	CB	CYS 481	37.429	33.058	19.155	1.00	12.24	BTKA
ATOM	656	SG	CYS 481	37.336	34.396	20.332	1.00	19.49	BTKA
ATOM	657	C	CYS 481	38.471	34.591	17.466	1.00	14.17	BTKA
ATOM	658	O	CYS 481	39.155	35.525	17.895	1.00	12.70	BTKA
ATOM	659	N	LEU 482	37.617	34.710	16.457	1.00	13.70	BTKA
ATOM	660	CA	LEU 482	37.419	35.940	15.711	1.00	14.10	BTKA
ATOM	661	CB	LEU 482	36.332	35.727	14.658	1.00	15.16	BTKA
ATOM	662	CG	LEU 482	35.978	36.880	13.718	1.00	15.54	BTKA
ATOM	663	CD1	LEU 482	37.163	37.237	12.839	1.00	13.49	BTKA
ATOM	664	CD2	LEU 482	34.792	36.478	12.866	1.00	11.61	BTKA
ATOM	665	C	LEU 482	37.042	37.100	16.620	1.00	13.30	BTKA
ATOM	666	O	LEU 482	37.436	38.235	16.371	1.00	11.50	BTKA
ATOM	667	N	LEU 483	36.283	36.816	17.674	1.00	14.77	BTKA
ATOM	668	CA	LEU 483	35.861	37.856	18.604	1.00	18.16	BTKA
ATOM	669	CB	LEU 483	34.949	37.266	19.682	1.00	16.94	BTKA
ATOM	670	CG	LEU 483	34.146	38.245	20.538	1.00	14.08	BTKA
ATOM	671	CD1	LEU 483	33.408	39.261	19.667	1.00	16.88	BTKA
ATOM	672	CD2	LEU 483	33.162	37.464	21.361	1.00	14.16	BTKA
ATOM	673	C	LEU 483	37.079	38.543	19.224	1.00	18.15	BTKA
ATOM	674	O	LEU 483	37.198	39.770	19.181	1.00	17.24	BTKA
ATOM	675	N	ASN 484	38.009	37.739	19.729	1.00	18.40	BTKA
ATOM	676	CA	ASN 484	39.238	38.239	20.340	1.00	17.40	BTKA
ATOM	677	CB	ASN 484	40.024	37.078	20.957	1.00	20.05	BTKA
ATOM	678	CG	ASN 484	41.426	37.474	21.390	1.00	22.96	BTKA
ATOM	679	OD1	ASN 484	41.687	38.628	21.741	1.00	27.75	BTKA
ATOM	680	ND2	ASN 484	42.338	36.511	21.374	1.00	26.58	BTKA
ATOM	681	C	ASN 484	40.086	38.925	19.286	1.00	16.06	BTKA
ATOM	682	O	ASN 484	40.682	39.971	19.535	1.00	22.07	BTKA
ATOM	683	N	TYR 485	40.101	38.350	18.092	1.00	13.87	BTKA
ATOM	684	CA	TYR 485	40.880	38.889	16.985	1.00	8.60	BTKA
ATOM	685	CB	TYR 485	40.775	37.944	15.791	1.00	5.86	BTKA
ATOM	686	CG	TYR 485	41.861	38.126	14.770	1.00	6.11	BTKA
ATOM	687	CD1	TYR 485	43.186	37.815	15.073	1.00	8.26	BTKA
ATOM	688	CE1	TYR 485	44.193	37.969	14.128	1.00	12.73	BTKA
ATOM	689	CD2	TYR 485	41.568	38.600	13.492	1.00	11.03	BTKA
ATOM	690	CE2	TYR 485	42.575	38.763	12.535	1.00	12.88	BTKA

	Atom Number	Atom Type	Amino Acid Residue		X	Y	Z	Occ.	Temp Factor	
ATOM	691	CZ	TYR	485	43.881	38.445	12.861	1.00	13.61	BTKA
ATOM	692	OH	TYR	485	44.873	38.605	11.920	1.00	19.94	BTKA
ATOM	693	C	TYR	485	40.432	40.296	16.587	1.00	9.48	BTKA
ATOM	694	O	TYR	485	41.250	41.203	16.394	1.00	8.68	BTKA
ATOM	695	N	LEU	486	39.121	40.472	16.516	1.00	8.14	BTKA
ATOM	696	CA	LEU	486	38.504	41.729	16.137	1.00	10.39	BTKA
ATOM	697	CB	LEU	486	36.996	41.521	15.971	1.00	7.77	BTKA
ATOM	698	CG	LEU	486	36.398	41.527	14.560	1.00	10.49	BTKA
ATOM	699	CD1	LEU	486	37.380	41.001	13.537	1.00	13.85	BTKA
ATOM	700	CD2	LEU	486	35.114	40.699	14.561	1.00	13.88	BTKA
ATOM	701	C	LEU	486	38.770	42.885	17.088	1.00	9.35	BTKA
ATOM	702	O	LEU	486	38.730	44.047	16.679	1.00	10.01	BTKA
ATOM	703	N	ARG	487	39.022	42.585	18.353	1.00	11.39	BTKA
ATOM	704	CA	ARG	487	39.269	43.634	19.337	1.00	13.42	BTKA
ATOM	705	CB	ARG	487	38.530	43.331	20.623	1.00	12.34	BTKA
ATOM	706	CG	ARG	487	37.048	43.342	20.498	1.00	6.56	BTKA
ATOM	707	CD	ARG	487	36.480	42.775	21.757	1.00	9.94	BTKA
ATOM	708	NE	ARG	487	35.036	42.696	21.683	1.00	10.94	BTKA
ATOM	709	CZ	ARG	487	34.323	41.676	22.134	1.00	8.89	BTKA
ATOM	710	NH1	ARG	487	34.917	40.631	22.700	1.00	8.34	BTKA
ATOM	711	NH2	ARG	487	33.004	41.715	22.036	1.00	6.96	BTKA
ATOM	712	C	ARG	487	40.718	43.882	19.691	1.00	15.16	BTKA
ATOM	713	O	ARG	487	41.069	45.007	20.043	1.00	15.60	BTKA
ATOM	714	N	GLU	488	41.542	42.835	19.625	1.00	21.25	BTKA
ATOM	715	CA	GLU	488	42.958	42.918	19.980	1.00	22.43	BTKA
ATOM	716	CB	GLU	488	43.576	41.513	20.072	1.00	20.93	BTKA
ATOM	717	CG	GLU	488	43.928	40.849	18.742	1.00	22.66	BTKA
ATOM	718	CD	GLU	488	44.657	39.525	18.926	1.00	25.51	BTKA
ATOM	719	OE1	GLU	488	45.809	39.523	19.417	1.00	25.84	BTKA
ATOM	720	OE2	GLU	488	44.072	38.476	18.590	1.00	29.76	BTKA
ATOM	721	C	GLU	488	43.813	43.825	19.095	1.00	24.56	BTKA
ATOM	722	O	GLU	488	43.294	44.710	18.418	1.00	24.48	BTKA
ATOM	723	N	MET	489	45.130	43.609	19.127	1.00	28.65	BTKA
ATOM	724	CA	MET	489	46.093	44.396	18.351	1.00	31.30	BTKA
ATOM	725	CB	MET	489	47.494	43.788	18.466	1.00	31.45	BTKA
ATOM	726	CG	MET	489	48.348	44.318	19.616	1.00	29.69	BTKA
ATOM	727	SD	MET	489	47.736	43.928	21.263	1.00	34.34	BTKA
ATOM	728	CE	MET	489	46.980	45.509	21.726	1.00	31.43	BTKA
ATOM	729	C	MET	489	45.736	44.554	16.880	1.00	31.31	BTKA
ATOM	730	O	MET	489	46.058	45.571	16.263	1.00	28.54	BTKA
ATOM	731	N	ARG	490	45.066	43.553	16.319	1.00	32.07	BTKA
ATOM	732	CA	ARG	490	44.671	43.593	14.914	1.00	31.59	BTKA
ATOM	733	CB	ARG	490	44.288	42.197	14.419	1.00	28.74	BTKA
ATOM	734	CG	ARG	490	45.454	41.270	14.138	1.00	27.20	BTKA
ATOM	735	CD	ARG	490	45.992	40.612	15.406	1.00	29.57	BTKA
ATOM	736	NE	ARG	490	47.097	41.349	16.016	1.00	30.05	BTKA
ATOM	737	CZ	ARG	490	48.120	40.767	16.631	1.00	25.67	BTKA
ATOM	738	NH1	ARG	490	48.180	39.446	16.723	1.00	24.51	BTKA
ATOM	739	NH2	ARG	490	49.098	41.505	17.129	1.00	26.01	BTKA
ATOM	740	C	ARG	490	43.524	44.567	14.632	1.00	31.84	BTKA
ATOM	741	O	ARG	490	43.181	44.797	13.475	1.00	31.98	BTKA
ATOM	742	N	HIS	491	42.977	45.166	15.688	1.00	31.55	BTKA
ATOM	743	CA	HIS	491	41.863	46.110	15.596	1.00	33.20	BTKA
ATOM	744	CB	HIS	491	41.770	46.937	16.885	1.00	33.15	BTKA
ATOM	745	CG	HIS	491	40.366	47.220	17.328	1.00	34.60	BTKA
ATOM	746	CD2	HIS	491	39.877	48.096	18.237	1.00	34.07	BTKA
ATOM	747	ND1	HIS	491	39.277	46.525	16.847	1.00	33.41	BTKA
ATOM	748	CE1	HIS	491	38.180	46.956	17.444	1.00	31.28	BTKA

Atom Number	Atom Type	Amino Acid Residue		X	Y	Z	Occ.	Temp Factor	
ATOM	749	NE2	HIS 491	38.517	47.909	18.292	1.00	32.75	BTKA
ATOM	750	C	HIS 491	41.927	47.055	14.401	1.00	35.09	BTKA
ATOM	751	O	HIS 491	40.892	47.404	13.828	1.00	37.68	BTKA
ATOM	752	N	ARG 492	43.136	47.484	14.046	1.00	34.42	BTKA
ATOM	753	CA	ARG 492	43.341	48.393	12.922	1.00	31.97	BTKA
ATOM	754	CB	ARG 492	44.726	49.047	13.013	1.00	33.81	BTKA
ATOM	755	CG	ARG 492	44.925	49.990	14.200	1.00	34.48	BTKA
ATOM	756	CD	ARG 492	44.943	49.258	15.537	1.00	35.35	BTKA
ATOM	757	NE	ARG 492	46.024	48.277	15.623	1.00	37.69	BTKA
ATOM	758	CZ	ARG 492	47.317	48.584	15.713	1.00	41.57	BTKA
ATOM	759	NH1	ARG 492	47.711	49.853	15.725	1.00	42.87	BTKA
ATOM	760	NH2	ARG 492	48.223	47.619	15.805	1.00	41.91	BTKA
ATOM	761	C	ARG 492	43.208	47.640	11.600	1.00	29.95	BTKA
ATOM	762	O	ARG 492	44.205	47.236	11.004	1.00	30.14	BTKA
ATOM	763	N	PHE 493	41.972	47.420	11.169	1.00	25.31	BTKA
ATOM	764	CA	PHE 493	41.722	46.704	9.927	1.00	25.42	BTKA
ATOM	765	CB	PHE 493	40.492	45.790	10.069	1.00	21.25	BTKA
ATOM	766	CG	PHE 493	40.713	44.585	10.943	1.00	20.61	BTKA
ATOM	767	CD1	PHE 493	41.466	43.508	10.488	1.00	19.35	BTKA
ATOM	768	CD2	PHE 493	40.151	44.518	12.215	1.00	18.30	BTKA
ATOM	769	CE1	PHE 493	41.656	42.382	11.290	1.00	19.86	BTKA
ATOM	770	CE2	PHE 493	40.335	43.396	13.024	1.00	18.27	BTKA
ATOM	771	CZ	PHE 493	41.084	42.328	12.565	1.00	14.30	BTKA
ATOM	772	C	PHE 493	41.532	47.663	8.751	1.00	28.44	BTKA
ATOM	773	O	PHE 493	42.235	48.669	8.625	1.00	28.08	BTKA
ATOM	774	N	GLN 494	40.585	47.315	7.884	1.00	28.76	BTKA
ATOM	775	CA	GLN 494	40.222	48.074	6.695	1.00	25.62	BTKA
ATOM	776	CB	GLN 494	41.401	48.139	5.723	1.00	26.48	BTKA
ATOM	777	CG	GLN 494	41.889	46.775	5.258	1.00	31.44	BTKA
ATOM	778	CD	GLN 494	43.164	46.832	4.437	1.00	31.26	BTKA
ATOM	779	OE1	GLN 494	43.411	45.961	3.598	1.00	31.88	BTKA
ATOM	780	NE2	GLN 494	43.989	47.846	4.679	1.00	31.84	BTKA
ATOM	781	C	GLN 494	39.082	47.251	6.098	1.00	23.81	BTKA
ATOM	782	O	GLN 494	39.051	46.032	6.270	1.00	22.09	BTKA
ATOM	783	N	THR 495	38.140	47.908	5.429	1.00	24.19	BTKA
ATOM	784	CA	THR 495	36.991	47.241	4.820	1.00	21.26	BTKA
ATOM	785	CB	THR 495	36.291	48.166	3.820	1.00	24.52	BTKA
ATOM	786	OG1	THR 495	36.242	49.495	4.352	1.00	28.48	BTKA
ATOM	787	CG2	THR 495	34.875	47.661	3.529	1.00	24.14	BTKA
ATOM	788	C	THR 495	37.376	45.978	4.061	1.00	18.91	BTKA
ATOM	789	O	THR 495	36.650	44.982	4.081	1.00	19.68	BTKA
ATOM	790	N	GLN 496	38.528	46.030	3.400	1.00	19.97	BTKA
ATOM	791	CA	GLN 496	39.026	44.915	2.612	1.00	19.83	BTKA
ATOM	792	CB	GLN 496	40.354	45.289	1.954	1.00	18.70	BTKA
ATOM	793	CG	GLN 496	40.198	46.264	0.789	1.00	23.77	BTKA
ATOM	794	CD	GLN 496	39.583	47.592	1.201	1.00	26.56	BTKA
ATOM	795	OE1	GLN 496	39.831	48.089	2.301	1.00	27.00	BTKA
ATOM	796	NE2	GLN 496	38.762	48.166	0.328	1.00	24.89	BTKA
ATOM	797	C	GLN 496	39.162	43.639	3.431	1.00	18.82	BTKA
ATOM	798	O	GLN 496	38.719	42.570	3.001	1.00	18.80	BTKA
ATOM	799	N	GLN 497	39.716	43.773	4.634	1.00	18.01	BTKA
ATOM	800	CA	GLN 497	39.910	42.644	5.542	1.00	16.28	BTKA
ATOM	801	CB	GLN 497	40.942	43.003	6.613	1.00	15.98	BTKA
ATOM	802	CG	GLN 497	42.329	43.311	6.059	1.00	16.87	BTKA
ATOM	803	CD	GLN 497	43.258	43.930	7.096	1.00	21.37	BTKA
ATOM	804	OE1	GLN 497	43.364	45.153	7.202	1.00	21.47	BTKA
ATOM	805	NE2	GLN 497	43.936	43.087	7.864	1.00	22.57	BTKA
ATOM	806	C	GLN 497	38.586	42.243	6.198	1.00	12.86	BTKA

Atom Number	Atom Type	Amino Acid Residue		X	Y	Z	Occ.	Temp Factor	
ATOM	807	O	GLN 497	38.377	41.085	6.546	1.00	10.95	BTKA
ATOM	808	N	LEU 498	37.683	43.202	6.342	1.00	10.21	BTKA
ATOM	809	CA	LEU 498	36.388	42.924	6.944	1.00	9.62	BTKA
ATOM	810	CB	LEU 498	35.682	44.230	7.306	1.00	10.33	BTKA
ATOM	811	CG	LEU 498	35.894	44.842	8.700	1.00	8.10	BTKA
ATOM	812	CD1	LEU 498	37.228	44.470	9.307	1.00	11.10	BTKA
ATOM	813	CD2	LEU 498	35.750	46.335	8.611	1.00	6.67	BTKA
ATOM	814	C	LEU 498	35.535	42.078	6.004	1.00	10.86	BTKA
ATOM	815	O	LEU 498	34.959	41.070	6.420	1.00	12.75	BTKA
ATOM	816	N	LEU 499	35.514	42.429	4.722	1.00	9.42	BTKA
ATOM	817	CA	LEU 499	34.725	41.661	3.764	1.00	11.87	BTKA
ATOM	818	CB	LEU 499	34.588	42.401	2.424	1.00	8.90	BTKA
ATOM	819	CG	LEU 499	33.332	42.005	1.634	1.00	9.18	BTKA
ATOM	820	CD1	LEU 499	32.100	42.507	2.347	1.00	4.94	BTKA
ATOM	821	CD2	LEU 499	33.371	42.551	0.226	1.00	9.87	BTKA
ATOM	822	C	LEU 499	35.327	40.270	3.548	1.00	12.95	BTKA
ATOM	823	O	LEU 499	34.592	39.287	3.410	1.00	16.98	BTKA
ATOM	824	N	GLU 500	36.658	40.190	3.515	1.00	13.94	BTKA
ATOM	825	CA	GLU 500	37.369	38.922	3.327	1.00	13.24	BTKA
ATOM	826	CB	GLU 500	38.887	39.150	3.415	1.00	16.16	BTKA
ATOM	827	CG	GLU 500	39.771	37.887	3.353	1.00	20.06	BTKA
ATOM	828	CD	GLU 500	39.721	37.146	2.016	1.00	22.89	BTKA
ATOM	829	OE1	GLU 500	39.841	35.901	2.032	1.00	26.56	BTKA
ATOM	830	OE2	GLU 500	39.571	37.791	0.953	1.00	24.13	BTKA
ATOM	831	C	GLU 500	36.923	37.909	4.377	1.00	10.91	BTKA
ATOM	832	O	GLU 500	36.671	36.739	4.068	1.00	10.95	BTKA
ATOM	833	N	MET 501	36.795	38.377	5.614	1.00	11.96	BTKA
ATOM	834	CA	MET 501	36.365	37.533	6.722	1.00	11.06	BTKA
ATOM	835	CB	MET 501	36.449	38.289	8.047	1.00	10.47	BTKA
ATOM	836	CG	MET 501	37.854	38.714	8.415	1.00	13.77	BTKA
ATOM	837	SD	MET 501	37.954	39.544	10.013	1.00	20.98	BTKA
ATOM	838	CE	MET 501	39.741	39.784	10.118	1.00	14.07	BTKA
ATOM	839	C	MET 501	34.947	37.032	6.503	1.00	9.64	BTKA
ATOM	840	O	MET 501	34.661	35.876	6.772	1.00	8.63	BTKA
ATOM	841	N	CYS 502	34.057	37.897	6.027	1.00	11.41	BTKA
ATOM	842	CA	CYS 502	32.676	37.493	5.768	1.00	13.88	BTKA
ATOM	843	CB	CYS 502	31.827	38.688	5.321	1.00	16.90	BTKA
ATOM	844	SG	CYS 502	31.751	40.046	6.496	1.00	14.48	BTKA
ATOM	845	C	CYS 502	32.642	36.410	4.688	1.00	12.88	BTKA
ATOM	846	O	CYS 502	31.844	35.473	4.763	1.00	14.89	BTKA
ATOM	847	N	LYS 503	33.508	36.552	3.688	1.00	13.23	BTKA
ATOM	848	CA	LYS 503	33.622	35.597	2.586	1.00	10.87	BTKA
ATOM	849	CB	LYS 503	34.606	36.132	1.539	1.00	12.02	BTKA
ATOM	850	CG	LYS 503	34.948	35.161	0.415	1.00	11.71	BTKA
ATOM	851	CD	LYS 503	35.937	35.789	-0.550	1.00	17.80	BTKA
ATOM	852	CE	LYS 503	36.351	34.811	-1.638	1.00	18.39	BTKA
ATOM	853	NZ	LYS 503	37.022	35.506	-2.763	1.00	19.21	BTKA
ATOM	854	C	LYS 503	34.082	34.224	3.095	1.00	10.24	BTKA
ATOM	855	O	LYS 503	33.471	33.203	2.765	1.00	9.05	BTKA
ATOM	856	N	ASP 504	35.131	34.204	3.921	1.00	10.68	BTKA
ATOM	857	CA	ASP 504	35.653	32.954	4.486	1.00	7.72	BTKA
ATOM	858	CB	ASP 504	36.748	33.229	5.530	1.00	8.01	BTKA
ATOM	859	CG	ASP 504	37.947	33.983	4.972	1.00	12.07	BTKA
ATOM	860	OD1	ASP 504	38.633	34.654	5.773	1.00	7.24	BTKA
ATOM	861	OD2	ASP 504	38.225	33.906	3.756	1.00	18.62	BTKA
ATOM	862	C	ASP 504	34.538	32.178	5.185	1.00	7.40	BTKA
ATOM	863	O	ASP 504	34.425	30.957	5.041	1.00	7.01	BTKA
ATOM	864	N	VAL 505	33.740	32.896	5.971	1.00	8.06	BTKA

	Atom Number	Atom Type	Amino Acid Residue		X	Y	Z	Occ.	Temp Factor	
ATOM	865	CA	VAL	505	32.640	32.302	6.726	1.00	6.77	BTKA
ATOM	866	CB	VAL	505	32.097	33.280	7.799	1.00	7.29	BTKA
ATOM	867	CG1	VAL	505	31.036	32.590	8.662	1.00	6.82	BTKA
ATOM	868	CG2	VAL	505	33.230	33.779	8.673	1.00	10.15	BTKA
ATOM	869	C	VAL	505	31.507	31.854	5.809	1.00	4.31	BTKA
ATOM	870	O	VAL	505	30.924	30.787	6.008	1.00	4.27	BTKA
ATOM	871	N	CYS	506	31.201	32.660	4.803	1.00	7.86	BTKA
ATOM	872	CA	CYS	506	30.144	32.331	3.847	1.00	8.57	BTKA
ATOM	873	CB	CYS	506	29.838	33.529	2.950	1.00	8.83	BTKA
ATOM	874	SG	CYS	506	28.173	33.501	2.267	1.00	9.16	BTKA
ATOM	875	C	CYS	506	30.531	31.120	2.987	1.00	8.76	BTKA
ATOM	876	O	CYS	506	29.668	30.406	2.479	1.00	8.42	BTKA
ATOM	877	N	GLU	507	31.831	30.904	2.810	1.00	9.14	BTKA
ATOM	878	CA	GLU	507	32.307	29.765	2.044	1.00	8.13	BTKA
ATOM	879	CB	GLU	507	33.786	29.915	1.707	1.00	7.62	BTKA
ATOM	880	CG	GLU	507	34.049	30.890	0.567	1.00	10.42	BTKA
ATOM	881	CD	GLU	507	35.508	30.972	0.200	1.00	8.86	BTKA
ATOM	882	OE1	GLU	507	35.807	31.383	-0.932	1.00	14.46	BTKA
ATOM	883	OE2	GLU	507	36.364	30.625	1.039	1.00	11.94	BTKA
ATOM	884	C	GLU	507	32.079	28.493	2.836	1.00	4.79	BTKA
ATOM	885	O	GLU	507	31.679	27.467	2.290	1.00	5.50	BTKA
ATOM	886	N	ALA	508	32.331	28.560	4.133	1.00	4.69	BTKA
ATOM	887	CA	ALA	508	32.132	27.411	5.003	1.00	2.84	BTKA
ATOM	888	CB	ALA	508	32.819	27.647	6.328	1.00	3.35	BTKA
ATOM	889	C	ALA	508	30.640	27.148	5.217	1.00	2.47	BTKA
ATOM	890	O	ALA	508	30.208	26.006	5.312	1.00	3.01	BTKA
ATOM	891	N	MET	509	29.851	28.214	5.261	1.00	4.27	BTKA
ATOM	892	CA	MET	509	28.415	28.096	5.459	1.00	3.24	BTKA
ATOM	893	CB	MET	509	27.829	29.434	5.905	1.00	2.63	BTKA
ATOM	894	CG	MET	509	28.209	29.825	7.328	1.00	5.18	BTKA
ATOM	895	SD	MET	509	27.764	28.538	8.519	1.00	12.83	BTKA
ATOM	896	CE	MET	509	29.227	28.333	9.323	1.00	11.58	BTKA
ATOM	897	C	MET	509	27.699	27.571	4.224	1.00	4.52	BTKA
ATOM	898	O	MET	509	26.794	26.748	4.333	1.00	8.63	BTKA
ATOM	899	N	GLU	510	28.094	28.057	3.050	1.00	5.93	BTKA
ATOM	900	CA	GLU	510	27.504	27.606	1.788	1.00	7.82	BTKA
ATOM	901	CB	GLU	510	28.167	28.327	0.615	1.00	7.50	BTKA
ATOM	902	CG	GLU	510	27.557	28.018	-0.737	1.00	18.01	BTKA
ATOM	903	CD	GLU	510	28.399	28.535	-1.898	1.00	21.81	BTKA
ATOM	904	OE1	GLU	510	27.811	28.919	-2.933	1.00	27.32	BTKA
ATOM	905	OE2	GLU	510	29.645	28.544	-1.781	1.00	24.20	BTKA
ATOM	906	C	GLU	510	27.719	26.090	1.671	1.00	5.58	BTKA
ATOM	907	O	GLU	510	26.811	25.347	1.292	1.00	5.09	BTKA
ATOM	908	N	TYR	511	28.918	25.643	2.049	1.00	7.55	BTKA
ATOM	909	CA	TYR	511	29.269	24.229	2.031	1.00	6.74	BTKA
ATOM	910	CB	TYR	511	30.748	24.049	2.400	1.00	9.67	BTKA
ATOM	911	CG	TYR	511	31.172	22.598	2.511	1.00	14.31	BTKA
ATOM	912	CD1	TYR	511	31.217	21.774	1.386	1.00	12.15	BTKA
ATOM	913	CE1	TYR	511	31.526	20.423	1.498	1.00	11.02	BTKA
ATOM	914	CD2	TYR	511	31.459	22.032	3.751	1.00	13.80	BTKA
ATOM	915	CE2	TYR	511	31.768	20.685	3.868	1.00	12.93	BTKA
ATOM	916	CZ	TYR	511	31.796	19.886	2.739	1.00	11.33	BTKA
ATOM	917	OH	TYR	511	32.057	18.545	2.875	1.00	14.81	BTKA
ATOM	918	C	TYR	511	28.368	23.405	2.975	1.00	8.27	BTKA
ATOM	919	O	TYR	511	27.916	22.316	2.611	1.00	8.84	BTKA
ATOM	920	N	LEU	512	28.121	23.907	4.184	1.00	8.72	BTKA
ATOM	921	CA	LEU	512	27.267	23.188	5.131	1.00	10.18	BTKA
ATOM	922	CB	LEU	512	27.232	23.878	6.503	1.00	4.04	BTKA

	Atom Number	Atom Type	Amino Acid Residue		X	Y	Z	Occ.	Temp Factor	
ATOM	923	CG	LEU	512	28.534	23.878	7.307	1.00	3.83	BTKA
ATOM	924	CD1	LEU	512	28.300	24.439	8.703	1.00	2.00	BTKA
ATOM	925	CD2	LEU	512	29.073	22.449	7.386	1.00	2.00	BTKA
ATOM	926	C	LEU	512	25.859	23.061	4.579	1.00	12.90	BTKA
ATOM	927	O	LEU	512	25.251	21.991	4.639	1.00	12.40	BTKA
ATOM	928	N	GLU	513	25.359	24.156	4.012	1.00	13.36	BTKA
ATOM	929	CA	GLU	513	24.028	24.197	3.428	1.00	11.85	BTKA
ATOM	930	CB	GLU	513	23.777	25.584	2.831	1.00	13.01	BTKA
ATOM	931	CG	GLU	513	22.368	25.822	2.284	1.00	10.82	BTKA
ATOM	932	CD	GLU	513	22.151	27.264	1.828	1.00	11.92	BTKA
ATOM	933	OE1	GLU	513	22.923	27.742	0.960	1.00	14.37	BTKA
ATOM	934	OE2	GLU	513	21.208	27.919	2.338	1.00	10.65	BTKA
ATOM	935	C	GLU	513	23.852	23.101	2.370	1.00	11.40	BTKA
ATOM	936	O	GLU	513	22.850	22.389	2.375	1.00	9.38	BTKA
ATOM	937	N	SER	514	24.848	22.932	1.502	1.00	13.91	BTKA
ATOM	938	CA	SER	514	24.785	21.915	0.453	1.00	15.43	BTKA
ATOM	939	CB	SER	514	25.916	22.109	-0.561	1.00	15.20	BTKA
ATOM	940	OG	SER	514	27.179	22.170	0.076	1.00	13.45	BTKA
ATOM	941	C	SER	514	24.834	20.500	1.024	1.00	17.44	BTKA
ATOM	942	O	SER	514	24.500	19.528	0.343	1.00	15.53	BTKA
ATOM	943	N	LYS	515	25.278	20.391	2.271	1.00	17.30	BTKA
ATOM	944	CA	LYS	515	25.371	19.107	2.943	1.00	12.99	BTKA
ATOM	945	CB	LYS	515	26.740	18.968	3.618	1.00	13.16	BTKA
ATOM	946	CG	LYS	515	27.920	18.997	2.643	1.00	13.40	BTKA
ATOM	947	CD	LYS	515	27.911	17.783	1.725	1.00	10.90	BTKA
ATOM	948	CE	LYS	515	29.045	17.846	0.731	1.00	9.83	BTKA
ATOM	949	NZ	LYS	515	29.193	16.567	-0.031	1.00	11.46	BTKA
ATOM	950	C	LYS	515	24.256	18.942	3.973	1.00	13.83	BTKA
ATOM	951	O	LYS	515	24.292	18.024	4.780	1.00	15.25	BTKA
ATOM	952	N	GLN	516	23.265	19.831	3.928	1.00	13.54	BTKA
ATOM	953	CA	GLN	516	22.120	19.814	4.848	1.00	15.50	BTKA
ATOM	954	CB	GLN	516	21.149	18.679	4.498	1.00	20.10	BTKA
ATOM	955	CG	GLN	516	20.481	18.812	3.128	1.00	27.83	BTKA
ATOM	956	CD	GLN	516	21.461	18.701	1.976	1.00	30.31	BTKA
ATOM	957	OE1	GLN	516	21.517	19.568	1.107	1.00	31.11	BTKA
ATOM	958	NE2	GLN	516	22.246	17.634	1.968	1.00	32.70	BTKA
ATOM	959	C	GLN	516	22.547	19.738	6.313	1.00	14.29	BTKA
ATOM	960	O	GLN	516	21.888	19.123	7.155	1.00	10.17	BTKA
ATOM	961	N	PHE	517	23.674	20.362	6.608	1.00	15.64	BTKA
ATOM	962	CA	PHE	517	24.192	20.388	7.963	1.00	16.92	BTKA
ATOM	963	CB	PHE	517	25.668	20.004	7.974	1.00	13.86	BTKA
ATOM	964	CG	PHE	517	26.230	19.814	9.349	1.00	14.42	BTKA
ATOM	965	CD1	PHE	517	26.109	18.589	9.996	1.00	20.02	BTKA
ATOM	966	CD2	PHE	517	26.888	20.851	9.994	1.00	13.85	BTKA
ATOM	967	CE1	PHE	517	26.639	18.398	11.267	1.00	22.95	BTKA
ATOM	968	CE2	PHE	517	27.421	20.673	11.262	1.00	18.84	BTKA
ATOM	969	CZ	PHE	517	27.297	19.442	11.901	1.00	23.12	BTKA
ATOM	970	C	PHE	517	24.022	21.814	8.458	1.00	19.46	BTKA
ATOM	971	O	PHE	517	24.510	22.758	7.830	1.00	20.11	BTKA
ATOM	972	N	LEU	518	23.293	21.986	9.551	1.00	18.01	BTKA
ATOM	973	CA	LEU	518	23.091	23.323	10.069	1.00	17.59	BTKA
ATOM	974	CB	LEU	518	21.604	23.598	10.328	1.00	15.17	BTKA
ATOM	975	CG	LEU	518	20.968	23.286	11.679	1.00	15.72	BTKA
ATOM	976	CD1	LEU	518	20.619	24.599	12.368	1.00	18.80	BTKA
ATOM	977	CD2	LEU	518	19.717	22.461	11.477	1.00	16.60	BTKA
ATOM	978	C	LEU	518	23.926	23.569	11.310	1.00	14.94	BTKA
ATOM	979	O	LEU	518	24.198	22.660	12.086	1.00	14.17	BTKA
ATOM	980	N	HIS	519	24.395	24.801	11.424	1.00	15.04	BTKA

Atom Number	Atom Type	Amino Acid Residue		X	Y	Z	Occ.	Temp Factor	
ATOM 981	CA	HIS	519	25.205	25.286	12.538	1.00	15.75	BTKA
ATOM 982	CB	HIS	519	26.276	26.213	11.970	1.00	13.52	BTKA
ATOM 983	CG	HIS	519	27.416	26.469	12.894	1.00	8.55	BTKA
ATOM 984	CD2	HIS	519	28.744	26.566	12.651	1.00	4.28	BTKA
ATOM 985	ND1	HIS	519	27.261	26.635	14.250	1.00	2.10	BTKA
ATOM 986	CE1	HIS	519	28.444	26.816	14.806	1.00	8.67	BTKA
ATOM 987	NE2	HIS	519	29.360	26.779	13.858	1.00	4.20	BTKA
ATOM 988	C	HIS	519	24.226	26.090	13.405	1.00	17.47	BTKA
ATOM 989	O	HIS	519	23.929	27.239	13.093	1.00	21.50	BTKA
ATOM 990	N	ARG	520	23.774	25.510	14.511	1.00	15.16	BTKA
ATOM 991	CA	ARG	520	22.785	26.156	15.382	1.00	15.58	BTKA
ATOM 992	CB	ARG	520	22.065	25.114	16.245	1.00	15.27	BTKA
ATOM 993	CG	ARG	520	21.823	23.780	15.555	1.00	18.29	BTKA
ATOM 994	CD	ARG	520	20.966	22.857	16.392	1.00	20.10	BTKA
ATOM 995	NE	ARG	520	21.449	22.725	17.769	1.00	27.27	BTKA
ATOM 996	CZ	ARG	520	22.581	22.124	18.127	1.00	27.89	BTKA
ATOM 997	NH1	ARG	520	23.378	21.592	17.215	1.00	27.36	BTKA
ATOM 998	NH2	ARG	520	22.904	22.038	19.408	1.00	25.47	BTKA
ATOM 999	C	ARG	520	23.294	27.261	16.290	1.00	16.19	BTKA
ATOM 1000	O	ARG	520	22.536	27.798	17.095	1.00	16.18	BTKA
ATOM 1001	N	ASP	521	24.557	27.635	16.141	1.00	16.78	BTKA
ATOM 1002	CA	ASP	521	25.128	28.669	16.992	1.00	14.05	BTKA
ATOM 1003	CB	ASP	521	25.668	28.023	18.278	1.00	14.95	BTKA
ATOM 1004	CG	ASP	521	26.067	29.042	19.330	1.00	13.62	BTKA
ATOM 1005	OD1	ASP	521	25.579	30.194	19.278	1.00	13.41	BTKA
ATOM 1006	OD2	ASP	521	26.875	28.681	20.209	1.00	8.70	BTKA
ATOM 1007	C	ASP	521	26.235	29.425	16.269	1.00	11.05	BTKA
ATOM 1008	O	ASP	521	27.409	29.277	16.583	1.00	10.26	BTKA
ATOM 1009	N	LEU	522	25.871	30.188	15.251	1.00	12.24	BTKA
ATOM 1010	CA	LEU	522	26.868	30.949	14.511	1.00	11.62	BTKA
ATOM 1011	CB	LEU	522	26.451	31.112	13.049	1.00	11.48	BTKA
ATOM 1012	CG	LEU	522	27.453	30.814	11.932	1.00	8.77	BTKA
ATOM 1013	CD1	LEU	522	26.970	31.571	10.728	1.00	8.36	BTKA
ATOM 1014	CD2	LEU	522	28.891	31.232	12.269	1.00	10.90	BTKA
ATOM 1015	C	LEU	522	27.017	32.325	15.149	1.00	12.66	BTKA
ATOM 1016	O	LEU	522	26.043	33.058	15.286	1.00	14.12	BTKA
ATOM 1017	N	ALA	523	28.237	32.657	15.544	1.00	13.37	BTKA
ATOM 1018	CA	ALA	523	28.546	33.941	16.157	1.00	13.35	BTKA
ATOM 1019	CB	ALA	523	28.169	33.934	17.639	1.00	6.92	BTKA
ATOM 1020	C	ALA	523	30.050	34.109	15.989	1.00	13.67	BTKA
ATOM 1021	O	ALA	523	30.743	33.138	15.661	1.00	14.16	BTKA
ATOM 1022	N	ALA	524	30.552	35.326	16.193	1.00	11.77	BTKA
ATOM 1023	CA	ALA	524	31.980	35.597	16.062	1.00	12.32	BTKA
ATOM 1024	CB	ALA	524	32.262	37.083	16.210	1.00	10.35	BTKA
ATOM 1025	C	ALA	524	32.771	34.809	17.091	1.00	13.86	BTKA
ATOM 1026	O	ALA	524	33.936	34.468	16.856	1.00	17.70	BTKA
ATOM 1027	N	ARG	525	32.143	34.541	18.237	1.00	13.11	BTKA
ATOM 1028	CA	ARG	525	32.779	33.780	19.302	1.00	13.31	BTKA
ATOM 1029	CB	ARG	525	31.873	33.692	20.533	1.00	14.94	BTKA
ATOM 1030	CG	ARG	525	30.736	32.687	20.422	1.00	16.14	BTKA
ATOM 1031	CD	ARG	525	30.031	32.492	21.751	1.00	13.88	BTKA
ATOM 1032	NE	ARG	525	29.478	33.746	22.255	1.00	21.28	BTKA
ATOM 1033	CZ	ARG	525	28.257	34.205	21.989	1.00	22.82	BTKA
ATOM 1034	NH1	ARG	525	27.425	33.522	21.210	1.00	24.36	BTKA
ATOM 1035	NH2	ARG	525	27.859	35.343	22.536	1.00	21.29	BTKA
ATOM 1036	C	ARG	525	33.112	32.369	18.833	1.00	13.03	BTKA
ATOM 1037	O	ARG	525	34.027	31.750	19.360	1.00	12.07	BTKA
ATOM 1038	N	ASN	526	32.361	31.873	17.849	1.00	11.96	BTKA

	Atom Number	Atom Type	Amino Acid Residue		X	Y	Z	Occ.	Temp Factor	
ATOM	1039	CA	ASN	526	32.559	30.533	17.314	1.00	10.29	BTKA
ATOM	1040	CB	ASN	526	31.225	29.871	16.985	1.00	8.11	BTKA
ATOM	1041	CG	ASN	526	30.715	29.039	18.119	1.00	9.90	BTKA
ATOM	1042	OD1	ASN	526	31.187	29.165	19.247	1.00	11.02	BTKA
ATOM	1043	ND2	ASN	526	29.761	28.167	17.836	1.00	15.50	BTKA
ATOM	1044	C	ASN	526	33.475	30.422	16.111	1.00	8.66	BTKA
ATOM	1045	O	ASN	526	33.639	29.341	15.560	1.00	10.60	BTKA
ATOM	1046	N	CYS	527	34.056	31.526	15.678	1.00	6.87	BTKA
ATOM	1047	CA	CYS	527	34.963	31.476	14.541	1.00	8.50	BTKA
ATOM	1048	CB	CYS	527	34.656	32.610	13.558	1.00	10.13	BTKA
ATOM	1049	SG	CYS	527	33.099	32.432	12.694	1.00	7.24	BTKA
ATOM	1050	C	CYS	527	36.377	31.610	15.081	1.00	9.42	BTKA
ATOM	1051	O	CYS	527	36.583	32.269	16.093	1.00	10.96	BTKA
ATOM	1052	N	LEU	528	37.331	30.948	14.439	1.00	9.95	BTKA
ATOM	1053	CA	LEU	528	38.732	30.998	14.854	1.00	7.80	BTKA
ATOM	1054	CB	LEU	528	39.222	29.602	15.262	1.00	8.09	BTKA
ATOM	1055	CG	LEU	528	38.507	28.876	16.411	1.00	4.85	BTKA
ATOM	1056	CD1	LEU	528	39.088	27.501	16.633	1.00	5.23	BTKA
ATOM	1057	CD2	LEU	528	38.623	29.682	17.687	1.00	12.77	BTKA
ATOM	1058	C	LEU	528	39.560	31.539	13.693	1.00	7.58	BTKA
ATOM	1059	O	LEU	528	39.130	31.474	12.533	1.00	8.42	BTKA
ATOM	1060	N	VAL	529	40.725	32.100	14.010	1.00	9.03	BTKA
ATOM	1061	CA	VAL	529	41.631	32.674	13.013	1.00	9.97	BTKA
ATOM	1062	CB	VAL	529	41.836	34.180	13.268	1.00	4.59	BTKA
ATOM	1063	CG1	VAL	529	42.609	34.802	12.122	1.00	3.83	BTKA
ATOM	1064	CG2	VAL	529	40.513	34.871	13.483	1.00	3.81	BTKA
ATOM	1065	C	VAL	529	43.003	32.008	13.107	1.00	11.90	BTKA
ATOM	1066	O	VAL	529	43.581	31.952	14.193	1.00	16.82	BTKA
ATOM	1067	N	ASN	530	43.524	31.492	11.993	1.00	15.54	BTKA
ATOM	1068	CA	ASN	530	44.839	30.849	12.016	1.00	16.52	BTKA
ATOM	1069	CB	ASN	530	44.975	29.783	10.918	1.00	15.67	BTKA
ATOM	1070	CG	ASN	530	44.676	30.312	9.512	1.00	17.17	BTKA
ATOM	1071	OD1	ASN	530	44.972	31.462	9.168	1.00	11.18	BTKA
ATOM	1072	ND2	ASN	530	44.111	29.448	8.683	1.00	15.71	BTKA
ATOM	1073	C	ASN	530	45.959	31.886	11.945	1.00	18.49	BTKA
ATOM	1074	O	ASN	530	45.688	33.074	12.064	1.00	23.10	BTKA
ATOM	1075	N	ASP	531	47.208	31.454	11.768	1.00	20.52	BTKA
ATOM	1076	CA	ASP	531	48.329	32.397	11.708	1.00	22.28	BTKA
ATOM	1077	CB	ASP	531	49.662	31.695	12.018	1.00	24.91	BTKA
ATOM	1078	CG	ASP	531	50.626	32.581	12.834	1.00	28.03	BTKA
ATOM	1079	OD1	ASP	531	50.883	32.262	14.019	1.00	25.89	BTKA
ATOM	1080	OD2	ASP	531	51.130	33.595	12.298	1.00	27.88	BTKA
ATOM	1081	C	ASP	531	48.403	33.141	10.370	1.00	24.22	BTKA
ATOM	1082	O	ASP	531	49.089	34.162	10.253	1.00	26.63	BTKA
ATOM	1083	N	GLN	532	47.693	32.636	9.365	1.00	22.72	BTKA
ATOM	1084	CA	GLN	532	47.663	33.279	8.052	1.00	21.96	BTKA
ATOM	1085	CB	GLN	532	47.438	32.255	6.933	1.00	25.06	BTKA
ATOM	1086	CG	GLN	532	48.588	31.275	6.710	1.00	29.08	BTKA
ATOM	1087	CD	GLN	532	48.653	30.189	7.765	1.00	32.01	BTKA
ATOM	1088	OE1	GLN	532	49.302	30.346	8.801	1.00	31.49	BTKA
ATOM	1089	NE2	GLN	532	47.971	29.080	7.509	1.00	34.18	BTKA
ATOM	1090	C	GLN	532	46.556	34.333	8.009	1.00	20.47	BTKA
ATOM	1091	O	GLN	532	46.376	35.018	6.998	1.00	19.50	BTKA
ATOM	1092	N	GLY	533	45.814	34.448	9.109	1.00	19.48	BTKA
ATOM	1093	CA	GLY	533	44.734	35.409	9.181	1.00	17.27	BTKA
ATOM	1094	C	GLY	533	43.434	34.858	8.632	1.00	16.09	BTKA
ATOM	1095	O	GLY	533	42.411	35.549	8.624	1.00	15.63	BTKA
ATOM	1096	N	VAL	534	43.462	33.606	8.186	1.00	14.60	BTKA

Atom Number	Atom Type	Amino Acid Residue		X	Y	Z	Occ.	Temp Factor	
ATOM 1097	CA	VAL	534	42.265	32.984	7.633	1.00	10.73	BTKA
ATOM 1098	CB	VAL	534	42.579	31.675	6.869	1.00	8.97	BTKA
ATOM 1099	CG1	VAL	534	41.299	31.097	6.283	1.00	10.35	BTKA
ATOM 1100	CG2	VAL	534	43.589	31.940	5.756	1.00	5.02	BTKA
ATOM 1101	C	VAL	534	41.257	32.719	8.744	1.00	6.19	BTKA
ATOM 1102	O	VAL	534	41.620	32.335	9.859	1.00	8.54	BTKA
ATOM 1103	N	VAL	535	39.998	32.994	8.440	1.00	7.49	BTKA
ATOM 1104	CA	VAL	535	38.915	32.820	9.385	1.00	6.02	BTKA
ATOM 1105	CB	VAL	535	37.918	34.028	9.338	1.00	5.47	BTKA
ATOM 1106	CG1	VAL	535	36.737	33.808	10.281	1.00	2.00	BTKA
ATOM 1107	CG2	VAL	535	38.632	35.308	9.725	1.00	4.76	BTKA
ATOM 1108	C	VAL	535	38.214	31.540	9.018	1.00	10.54	BTKA
ATOM 1109	O	VAL	535	37.929	31.283	7.840	1.00	11.45	BTKA
ATOM 1110	N	LYS	536	37.985	30.714	10.029	1.00	13.48	BTKA
ATOM 1111	CA	LYS	536	37.314	29.440	9.841	1.00	10.58	BTKA
ATOM 1112	CB	LYS	536	38.303	28.286	10.030	1.00	7.32	BTKA
ATOM 1113	CG	LYS	536	39.494	28.342	9.113	1.00	2.94	BTKA
ATOM 1114	CD	LYS	536	40.172	26.996	9.009	1.00	2.00	BTKA
ATOM 1115	CE	LYS	536	41.398	27.103	8.113	1.00	8.60	BTKA
ATOM 1116	NZ	LYS	536	41.911	25.779	7.679	1.00	8.95	BTKA
ATOM 1117	C	LYS	536	36.194	29.328	10.863	1.00	11.55	BTKA
ATOM 1118	O	LYS	536	36.291	29.859	11.972	1.00	13.24	BTKA
ATOM 1119	N	VAL	537	35.112	28.673	10.481	1.00	12.34	BTKA
ATOM 1120	CA	VAL	537	34.000	28.503	11.395	1.00	10.90	BTKA
ATOM 1121	CB	VAL	537	32.635	28.484	10.649	1.00	11.82	BTKA
ATOM 1122	CG1	VAL	537	32.547	29.644	9.678	1.00	5.08	BTKA
ATOM 1123	CG2	VAL	537	32.439	27.188	9.923	1.00	8.05	BTKA
ATOM 1124	C	VAL	537	34.216	27.200	12.165	1.00	8.75	BTKA
ATOM 1125	O	VAL	537	34.718	26.220	11.623	1.00	4.07	BTKA
ATOM 1126	N	SER	538	33.850	27.191	13.436	1.00	8.53	BTKA
ATOM 1127	CA	SER	538	34.023	26.004	14.244	1.00	9.45	BTKA
ATOM 1128	CB	SER	538	35.286	26.161	15.091	1.00	12.59	BTKA
ATOM 1129	OG	SER	538	35.492	27.515	15.458	1.00	17.47	BTKA
ATOM 1130	C	SER	538	32.810	25.733	15.121	1.00	10.31	BTKA
ATOM 1131	O	SER	538	31.716	26.215	14.844	1.00	6.08	BTKA
ATOM 1132	N	ASP	539	33.005	24.916	16.150	1.00	15.14	BTKA
ATOM 1133	CA	ASP	539	31.962	24.551	17.096	1.00	16.76	BTKA
ATOM 1134	CB	ASP	539	31.806	25.633	18.170	1.00	18.57	BTKA
ATOM 1135	CG	ASP	539	32.995	25.693	19.113	1.00	21.43	BTKA
ATOM 1136	OD1	ASP	539	33.900	24.834	18.995	1.00	22.15	BTKA
ATOM 1137	OD2	ASP	539	33.025	26.597	19.975	1.00	22.92	BTKA
ATOM 1138	C	ASP	539	30.614	24.162	16.488	1.00	17.48	BTKA
ATOM 1139	O	ASP	539	29.555	24.628	16.912	1.00	16.42	BTKA
ATOM 1140	N	PHE	540	30.674	23.321	15.462	1.00	16.99	BTKA
ATOM 1141	CA	PHE	540	29.475	22.810	14.814	1.00	16.89	BTKA
ATOM 1142	CB	PHE	540	29.500	23.037	13.294	1.00	16.17	BTKA
ATOM 1143	CG	PHE	540	30.740	22.539	12.615	1.00	13.71	BTKA
ATOM 1144	CD1	PHE	540	31.805	23.397	12.371	1.00	16.51	BTKA
ATOM 1145	CD2	PHE	540	30.845	21.216	12.206	1.00	15.68	BTKA
ATOM 1146	CE1	PHE	540	32.961	22.945	11.729	1.00	16.66	BTKA
ATOM 1147	CE2	PHE	540	31.992	20.757	11.565	1.00	17.77	BTKA
ATOM 1148	CZ	PHE	540	33.053	21.626	11.327	1.00	15.13	BTKA
ATOM 1149	C	PHE	540	29.408	21.326	15.143	1.00	21.34	BTKA
ATOM 1150	O	PHE	540	28.789	20.547	14.428	1.00	23.74	BTKA
ATOM 1151	N	GLY	541	30.058	20.948	16.240	1.00	26.85	BTKA
ATOM 1152	CA	GLY	541	30.077	19.561	16.665	1.00	29.31	BTKA
ATOM 1153	C	GLY	541	28.691	19.006	16.891	1.00	30.12	BTKA
ATOM 1154	O	GLY	541	28.263	18.096	16.195	1.00	34.04	BTKA

	Atom Number	Atom Type	Amino Acid Residue		X	Y	Z	Occ.	Temp Factor	
ATOM	1155	N	LEU	542	27.977	19.593	17.843	1.00	33.66	BTKA
ATOM	1156	CA	LEU	542	26.624	19.162	18.176	1.00	35.98	BTKA
ATOM	1157	CB	LEU	542	26.172	19.825	19.477	1.00	34.47	BTKA
ATOM	1158	CG	LEU	542	24.945	19.203	20.138	1.00	32.57	BTKA
ATOM	1159	CD1	LEU	542	25.249	17.747	20.483	1.00	31.46	BTKA
ATOM	1160	CD2	LEU	542	24.570	19.988	21.384	1.00	34.75	BTKA
ATOM	1161	C	LEU	542	25.611	19.465	17.073	1.00	37.74	BTKA
ATOM	1162	O	LEU	542	24.484	18.974	17.115	1.00	41.14	BTKA
ATOM	1163	N	SER	543	25.998	20.302	16.113	1.00	39.87	BTKA
ATOM	1164	CA	SER	543	25.119	20.670	15.006	1.00	37.74	BTKA
ATOM	1165	CB	SER	543	25.884	21.503	13.991	1.00	36.22	BTKA
ATOM	1166	OG	SER	543	26.286	22.741	14.549	1.00	39.50	BTKA
ATOM	1167	C	SER	543	24.500	19.438	14.353	1.00	36.64	BTKA
ATOM	1168	O	SER	543	25.122	18.378	14.295	1.00	39.71	BTKA
ATOM	1169	N	ARG	544	23.291	19.588	13.823	1.00	35.36	BTKA
ATOM	1170	CA	ARG	544	22.586	18.449	13.243	1.00	35.31	BTKA
ATOM	1171	CB	ARG	544	21.158	18.375	13.812	1.00	33.92	BTKA
ATOM	1172	CG	ARG	544	21.042	18.446	15.337	1.00	31.74	BTKA
ATOM	1173	CD	ARG	544	21.624	17.217	16.023	1.00	31.10	BTKA
ATOM	1174	NE	ARG	544	21.323	17.206	17.455	1.00	28.02	BTKA
ATOM	1175	CZ	ARG	544	22.167	16.789	18.394	1.00	27.42	BTKA
ATOM	1176	NH1	ARG	544	23.374	16.347	18.063	1.00	29.84	BTKA
ATOM	1177	NH2	ARG	544	21.803	16.809	19.669	1.00	24.16	BTKA
ATOM	1178	C	ARG	544	22.490	18.345	11.726	1.00	34.69	BTKA
ATOM	1179	O	ARG	544	22.040	19.275	11.050	1.00	34.23	BTKA
ATOM	1180	N	TYR	545	22.900	17.195	11.196	1.00	34.38	BTKA
ATOM	1181	CA	TYR	545	22.771	16.931	9.772	1.00	33.59	BTKA
ATOM	1182	CB	TYR	545	23.675	15.769	9.337	1.00	30.93	BTKA
ATOM	1183	CG	TYR	545	23.699	15.529	7.834	1.00	33.42	BTKA
ATOM	1184	CD1	TYR	545	22.515	15.298	7.120	1.00	31.23	BTKA
ATOM	1185	CE1	TYR	545	22.530	15.081	5.743	1.00	28.45	BTKA
ATOM	1186	CD2	TYR	545	24.904	15.531	7.125	1.00	28.39	BTKA
ATOM	1187	CE2	TYR	545	24.927	15.314	5.743	1.00	28.97	BTKA
ATOM	1188	CZ	TYR	545	23.735	15.089	5.059	1.00	28.78	BTKA
ATOM	1189	OH	TYR	545	23.743	14.896	3.694	1.00	25.38	BTKA
ATOM	1190	C	TYR	545	21.303	16.510	9.724	1.00	35.39	BTKA
ATOM	1191	O	TYR	545	20.970	15.333	9.879	1.00	37.41	BTKA
ATOM	1192	N	VAL	546	20.428	17.498	9.602	1.00	37.55	BTKA
ATOM	1193	CA	VAL	546	18.990	17.264	9.584	1.00	37.08	BTKA
ATOM	1194	CB	VAL	546	18.229	18.544	10.010	1.00	37.41	BTKA
ATOM	1195	CG1	VAL	546	16.764	18.249	10.197	1.00	37.58	BTKA
ATOM	1196	CG2	VAL	546	18.810	19.090	11.301	1.00	35.82	BTKA
ATOM	1197	C	VAL	546	18.493	16.787	8.224	1.00	37.83	BTKA
ATOM	1198	O	VAL	546	18.579	17.512	7.235	1.00	39.72	BTKA
ATOM	1199	N	LEU	547	17.979	15.561	8.183	1.00	38.29	BTKA
ATOM	1200	CA	LEU	547	17.464	14.983	6.942	1.00	38.05	BTKA
ATOM	1201	CB	LEU	547	17.040	13.525	7.145	1.00	36.02	BTKA
ATOM	1202	CG	LEU	547	18.080	12.537	7.681	1.00	37.29	BTKA
ATOM	1203	CD1	LEU	547	18.006	12.487	9.203	1.00	36.45	BTKA
ATOM	1204	CD2	LEU	547	17.816	11.151	7.105	1.00	41.49	BTKA
ATOM	1205	C	LEU	547	16.279	15.781	6.421	1.00	37.96	BTKA
ATOM	1206	O	LEU	547	16.163	16.022	5.226	1.00	39.78	BTKA
ATOM	1207	N	ASP	548	15.392	16.174	7.328	1.00	39.49	BTKA
ATOM	1208	CA	ASP	548	14.213	16.947	6.961	1.00	38.62	BTKA
ATOM	1209	CB	ASP	548	13.035	16.609	7.893	1.00	39.75	BTKA
ATOM	1210	CG	ASP	548	13.449	16.453	9.347	1.00	35.16	BTKA
ATOM	1211	OD1	ASP	548	13.389	15.323	9.871	1.00	35.03	BTKA
ATOM	1212	OD2	ASP	548	13.823	17.458	9.974	1.00	34.37	BTKA

Atom Number	Atom Type	Amino Acid Residue		X	Y	Z	Occ.	Temp Factor	
ATOM 1213	C	ASP	548	14.523	18.444	6.963	1.00	37.92	BTKA
ATOM 1214	O	ASP	548	15.281	18.921	7.799	1.00	39.58	BTKA
ATOM 1215	N	ASP	549	13.945	19.177	6.017	1.00	37.16	BTKA
ATOM 1216	CA	ASP	549	14.182	20.621	5.904	1.00	37.60	BTKA
ATOM 1217	CB	ASP	549	13.639	21.165	4.571	1.00	29.74	BTKA
ATOM 1218	CG	ASP	549	12.463	20.366	4.046	1.00	24.70	BTKA
ATOM 1219	OD1	ASP	549	11.311	20.721	4.369	1.00	21.17	BTKA
ATOM 1220	OD2	ASP	549	12.696	19.376	3.316	1.00	21.37	BTKA
ATOM 1221	C	ASP	549	13.715	21.492	7.081	1.00	39.63	BTKA
ATOM 1222	O	ASP	549	14.267	22.570	7.318	1.00	38.62	BTKA
ATOM 1223	N	GLU	550	12.692	21.042	7.800	1.00	42.46	BTKA
ATOM 1224	CA	GLU	550	12.183	21.783	8.951	1.00	43.87	BTKA
ATOM 1225	CB	GLU	550	10.653	21.676	9.014	1.00	44.48	BTKA
ATOM 1226	CG	GLU	550	9.950	22.690	9.924	1.00	42.81	BTKA
ATOM 1227	CD	GLU	550	10.269	22.514	11.401	1.00	43.82	BTKA
ATOM 1228	OE1	GLU	550	9.910	21.468	11.986	1.00	41.82	BTKA
ATOM 1229	OE2	GLU	550	10.884	23.428	11.984	1.00	43.35	BTKA
ATOM 1230	C	GLU	550	12.811	21.061	10.132	1.00	44.39	BTKA
ATOM 1231	O	GLU	550	12.798	19.833	10.161	1.00	45.16	BTKA
ATOM 1232	N	TYR	551	13.383	21.803	11.080	1.00	44.30	BTKA
ATOM 1233	CA	TYR	551	14.026	21.184	12.239	1.00	42.30	BTKA
ATOM 1234	CB	TYR	551	15.516	21.535	12.282	1.00	41.57	BTKA
ATOM 1235	CG	TYR	551	16.221	21.112	13.559	1.00	42.35	BTKA
ATOM 1236	CD1	TYR	551	16.573	19.780	13.786	1.00	43.14	BTKA
ATOM 1237	CE1	TYR	551	17.241	19.402	14.952	1.00	40.79	BTKA
ATOM 1238	CD2	TYR	551	16.550	22.051	14.533	1.00	40.74	BTKA
ATOM 1239	CE2	TYR	551	17.214	21.683	15.697	1.00	38.38	BTKA
ATOM 1240	CZ	TYR	551	17.555	20.365	15.902	1.00	39.27	BTKA
ATOM 1241	OH	TYR	551	18.206	20.021	17.061	1.00	41.15	BTKA
ATOM 1242	C	TYR	551	13.384	21.501	13.586	1.00	43.53	BTKA
ATOM 1243	O	TYR	551	12.965	22.633	13.849	1.00	41.79	BTKA
ATOM 1244	N	THR	552	13.329	20.475	14.431	1.00	44.17	BTKA
ATOM 1245	CA	THR	552	12.777	20.559	15.777	1.00	42.48	BTKA
ATOM 1246	CB	THR	552	11.555	19.626	15.927	1.00	40.83	BTKA
ATOM 1247	OG1	THR	552	11.850	18.351	15.345	1.00	39.32	BTKA
ATOM 1248	CG2	THR	552	10.343	20.216	15.226	1.00	40.05	BTKA
ATOM 1249	C	THR	552	13.900	20.118	16.716	1.00	43.93	BTKA
ATOM 1250	O	THR	552	14.784	19.366	16.300	1.00	45.33	BTKA
ATOM 1251	N	SER	553	13.884	20.584	17.963	1.00	42.56	BTKA
ATOM 1252	CA	SER	553	14.940	20.231	18.909	1.00	41.52	BTKA
ATOM 1253	CB	SER	553	15.942	21.388	18.998	1.00	43.12	BTKA
ATOM 1254	OG	SER	553	17.207	20.961	19.479	1.00	42.78	BTKA
ATOM 1255	C	SER	553	14.384	19.902	20.299	1.00	41.75	BTKA
ATOM 1256	O	SER	553	13.185	19.638	20.446	1.00	41.54	BTKA
ATOM 1257	N	SER	554	15.269	19.863	21.296	1.00	40.52	BTKA
ATOM 1258	CA	SER	554	14.883	19.589	22.678	1.00	41.03	BTKA
ATOM 1259	CB	SER	554	15.895	18.655	23.349	1.00	41.04	BTKA
ATOM 1260	OG	SER	554	15.346	18.053	24.515	1.00	41.68	BTKA
ATOM 1261	C	SER	554	14.833	20.932	23.406	1.00	41.29	BTKA
ATOM 1262	O	SER	554	13.833	21.273	24.033	1.00	40.26	BTKA
ATOM 1263	N	VAL	555	15.928	21.681	23.287	1.00	42.31	BTKA
ATOM 1264	CA	VAL	555	16.104	23.024	23.858	1.00	44.31	BTKA
ATOM 1265	CB	VAL	555	15.284	24.090	23.082	1.00	46.09	BTKA
ATOM 1266	CG1	VAL	555	15.359	23.808	21.607	1.00	45.26	BTKA
ATOM 1267	CG2	VAL	555	13.840	24.159	23.568	1.00	46.08	BTKA
ATOM 1268	C	VAL	555	15.979	23.284	25.365	1.00	43.78	BTKA
ATOM 1269	O	VAL	555	15.291	22.570	26.101	1.00	43.91	BTKA
ATOM 1270	N	GLY	556	16.690	24.324	25.797	1.00	42.58	BTKA

	Atom Number	Atom Type	Amino Acid Residue		X	Y	Z	Occ.	Temp Factor	
ATOM	1271	CA	GLY	556	16.712	24.732	27.187	1.00	42.48	BTKA
ATOM	1272	C	GLY	556	18.047	25.357	27.556	1.00	41.57	BTKA
ATOM	1273	O	GLY	556	18.784	25.812	26.675	1.00	41.16	BTKA
ATOM	1274	N	SER	557	18.352	25.378	28.853	1.00	40.73	BTKA
ATOM	1275	CA	SER	557	19.603	25.934	29.383	1.00	38.88	BTKA
ATOM	1276	CB	SER	557	20.812	25.220	28.764	1.00	40.14	BTKA
ATOM	1277	OG	SER	557	20.724	23.812	28.944	1.00	36.05	BTKA
ATOM	1278	C	SER	557	19.721	27.453	29.214	1.00	38.15	BTKA
ATOM	1279	O	SER	557	19.729	28.193	30.197	1.00	37.76	BTKA
ATOM	1280	N	LYS	558	19.826	27.905	27.971	1.00	36.40	BTKA
ATOM	1281	CA	LYS	558	19.926	29.323	27.648	1.00	33.00	BTKA
ATOM	1282	CB	LYS	558	21.170	29.948	28.284	1.00	32.93	BTKA
ATOM	1283	CG	LYS	558	21.234	31.480	28.249	1.00	28.95	BTKA
ATOM	1284	CD	LYS	558	20.109	32.151	29.034	1.00	25.19	BTKA
ATOM	1285	CE	LYS	558	18.864	32.378	28.182	1.00	24.86	BTKA
ATOM	1286	NZ	LYS	558	19.140	33.238	26.987	1.00	27.50	BTKA
ATOM	1287	C	LYS	558	19.987	29.415	26.127	1.00	32.13	BTKA
ATOM	1288	O	LYS	558	20.184	28.403	25.448	1.00	31.90	BTKA
ATOM	1289	N	PHE	559	19.843	30.618	25.591	1.00	31.72	BTKA
ATOM	1290	CA	PHE	559	19.848	30.797	24.147	1.00	30.24	BTKA
ATOM	1291	CB	PHE	559	18.410	31.033	23.671	1.00	33.13	BTKA
ATOM	1292	CG	PHE	559	18.028	30.265	22.440	1.00	36.97	BTKA
ATOM	1293	CD1	PHE	559	18.976	29.572	21.698	1.00	37.84	BTKA
ATOM	1294	CD2	PHE	559	16.697	30.207	22.042	1.00	40.25	BTKA
ATOM	1295	CE1	PHE	559	18.605	28.832	20.582	1.00	36.42	BTKA
ATOM	1296	CE2	PHE	559	16.318	29.468	20.932	1.00	39.23	BTKA
ATOM	1297	CZ	PHE	559	17.275	28.779	20.203	1.00	39.57	BTKA
ATOM	1298	C	PHE	559	20.672	32.005	23.738	1.00	28.68	BTKA
ATOM	1299	O	PHE	559	20.647	33.036	24.418	1.00	32.43	BTKA
ATOM	1300	N	PRO	560	21.505	31.859	22.696	1.00	25.69	BTKA
ATOM	1301	CD	PRO	560	21.989	30.606	22.090	1.00	23.07	BTKA
ATOM	1302	CA	PRO	560	22.303	33.003	22.244	1.00	25.30	BTKA
ATOM	1303	CB	PRO	560	23.371	32.343	21.371	1.00	24.23	BTKA
ATOM	1304	CG	PRO	560	22.695	31.103	20.873	1.00	23.44	BTKA
ATOM	1305	C	PRO	560	21.322	33.869	21.439	1.00	22.00	BTKA
ATOM	1306	O	PRO	560	21.428	34.002	20.220	1.00	20.54	BTKA
ATOM	1307	N	VAL	561	20.370	34.447	22.170	1.00	18.60	BTKA
ATOM	1308	CA	VAL	561	19.271	35.271	21.653	1.00	15.90	BTKA
ATOM	1309	CB	VAL	561	18.475	35.908	22.840	1.00	13.27	BTKA
ATOM	1310	CG1	VAL	561	17.202	36.587	22.348	1.00	12.23	BTKA
ATOM	1311	CG2	VAL	561	18.126	34.848	23.858	1.00	10.66	BTKA
ATOM	1312	C	VAL	561	19.631	36.360	20.645	1.00	12.76	BTKA
ATOM	1313	O	VAL	561	18.900	36.595	19.686	1.00	14.28	BTKA
ATOM	1314	N	ARG	562	20.778	36.990	20.849	1.00	11.30	BTKA
ATOM	1315	CA	ARG	562	21.238	38.078	19.996	1.00	7.17	BTKA
ATOM	1316	CB	ARG	562	22.435	38.756	20.647	1.00	6.00	BTKA
ATOM	1317	CG	ARG	562	22.184	39.160	22.086	1.00	7.62	BTKA
ATOM	1318	CD	ARG	562	23.396	39.859	22.678	1.00	8.88	BTKA
ATOM	1319	NE	ARG	562	23.231	40.134	24.100	1.00	12.40	BTKA
ATOM	1320	CZ	ARG	562	22.311	40.944	24.614	1.00	6.84	BTKA
ATOM	1321	NH1	ARG	562	22.250	41.118	25.921	1.00	15.72	BTKA
ATOM	1322	NH2	ARG	562	21.458	41.583	23.835	1.00	7.47	BTKA
ATOM	1323	C	ARG	562	21.587	37.696	18.569	1.00	8.37	BTKA
ATOM	1324	O	ARG	562	21.885	38.566	17.763	1.00	7.58	BTKA
ATOM	1325	N	TRP	563	21.584	36.402	18.264	1.00	9.41	BTKA
ATOM	1326	CA	TRP	563	21.909	35.920	16.918	1.00	7.23	BTKA
ATOM	1327	CB	TRP	563	23.207	35.107	16.932	1.00	7.42	BTKA
ATOM	1328	CG	TRP	563	24.422	35.878	17.243	1.00	6.68	BTKA

	Atom Number	Atom Type	Amino Acid Residue		X	Y	Z	Occ.	Temp Factor	
ATOM	1329	CD2	TRP	563	24.892	36.249	18.541	1.00	8.73	BTKA
ATOM	1330	CE2	TRP	563	26.070	36.995	18.358	1.00	8.54	BTKA
ATOM	1331	CE3	TRP	563	24.432	36.021	19.845	1.00	7.52	BTKA
ATOM	1332	CD1	TRP	563	25.306	36.388	16.351	1.00	10.62	BTKA
ATOM	1333	NE1	TRP	563	26.297	37.071	17.010	1.00	11.83	BTKA
ATOM	1334	CZ2	TRP	563	26.796	37.525	19.423	1.00	10.18	BTKA
ATOM	1335	CZ3	TRP	563	25.153	36.549	20.907	1.00	14.27	BTKA
ATOM	1336	CH2	TRP	563	26.325	37.292	20.686	1.00	11.16	BTKA
ATOM	1337	C	TRP	563	20.806	35.000	16.434	1.00	3.39	BTKA
ATOM	1338	O	TRP	563	20.986	34.269	15.470	1.00	6.67	BTKA
ATOM	1339	N	SER	564	19.654	35.063	17.080	1.00	4.53	BTKA
ATOM	1340	CA	SER	564	18.568	34.179	16.724	1.00	7.96	BTKA
ATOM	1341	CB	SER	564	18.134	33.404	17.971	1.00	9.14	BTKA
ATOM	1342	OG	SER	564	19.237	32.702	18.549	1.00	15.71	BTKA
ATOM	1343	C	SER	564	17.364	34.853	16.088	1.00	9.34	BTKA
ATOM	1344	O	SER	564	16.952	35.938	16.501	1.00	8.42	BTKA
ATOM	1345	N	PRO	565	16.839	34.255	15.004	1.00	9.83	BTKA
ATOM	1346	CD	PRO	565	17.389	33.137	14.219	1.00	10.36	BTKA
ATOM	1347	CA	PRO	565	15.671	34.821	14.336	1.00	11.63	BTKA
ATOM	1348	CB	PRO	565	15.605	34.018	13.033	1.00	7.64	BTKA
ATOM	1349	CG	PRO	565	16.203	32.723	13.395	1.00	3.54	BTKA
ATOM	1350	C	PRO	565	14.451	34.575	15.225	1.00	11.02	BTKA
ATOM	1351	O	PRO	565	14.444	33.649	16.040	1.00	9.72	BTKA
ATOM	1352	N	PRO	566	13.397	35.382	15.064	1.00	14.93	BTKA
ATOM	1353	CD	PRO	566	13.208	36.466	14.085	1.00	16.14	BTKA
ATOM	1354	CA	PRO	566	12.194	35.207	15.881	1.00	14.83	BTKA
ATOM	1355	CB	PRO	566	11.217	36.217	15.272	1.00	14.50	BTKA
ATOM	1356	CG	PRO	566	11.729	36.426	13.876	1.00	18.85	BTKA
ATOM	1357	C	PRO	566	11.617	33.781	15.963	1.00	12.73	BTKA
ATOM	1358	O	PRO	566	11.195	33.361	17.038	1.00	13.91	BTKA
ATOM	1359	N	GLU	567	11.636	33.012	14.874	1.00	13.43	BTKA
ATOM	1360	CA	GLU	567	11.075	31.652	14.932	1.00	13.41	BTKA
ATOM	1361	CB	GLU	567	10.789	31.072	13.541	1.00	15.94	BTKA
ATOM	1362	CG	GLU	567	12.010	30.662	12.730	1.00	17.33	BTKA
ATOM	1363	CD	GLU	567	12.733	31.825	12.072	1.00	12.50	BTKA
ATOM	1364	OE1	GLU	567	12.300	32.993	12.211	1.00	10.98	BTKA
ATOM	1365	OE2	GLU	567	13.749	31.550	11.404	1.00	9.50	BTKA
ATOM	1366	C	GLU	567	11.908	30.685	15.769	1.00	11.95	BTKA
ATOM	1367	O	GLU	567	11.460	29.581	16.106	1.00	12.58	BTKA
ATOM	1368	N	VAL	568	13.134	31.083	16.078	1.00	10.44	BTKA
ATOM	1369	CA	VAL	568	13.994	30.274	16.926	1.00	9.53	BTKA
ATOM	1370	CB	VAL	568	15.473	30.421	16.541	1.00	4.21	BTKA
ATOM	1371	CG1	VAL	568	16.331	30.518	17.751	1.00	6.04	BTKA
ATOM	1372	CG2	VAL	568	15.902	29.228	15.729	1.00	5.60	BTKA
ATOM	1373	C	VAL	568	13.722	30.798	18.331	1.00	10.51	BTKA
ATOM	1374	O	VAL	568	13.608	30.029	19.285	1.00	9.31	BTKA
ATOM	1375	N	LEU	569	13.521	32.110	18.415	1.00	10.75	BTKA
ATOM	1376	CA	LEU	569	13.218	32.803	19.663	1.00	14.44	BTKA
ATOM	1377	CB	LEU	569	13.137	34.308	19.397	1.00	12.26	BTKA
ATOM	1378	CG	LEU	569	14.207	35.247	19.958	1.00	11.89	BTKA
ATOM	1379	CD1	LEU	569	15.591	34.631	19.852	1.00	11.36	BTKA
ATOM	1380	CD2	LEU	569	14.135	36.583	19.221	1.00	12.38	BTKA
ATOM	1381	C	LEU	569	11.885	32.333	20.244	1.00	17.10	BTKA
ATOM	1382	O	LEU	569	11.709	32.288	21.462	1.00	20.31	BTKA
ATOM	1383	N	MET	570	10.959	31.964	19.363	1.00	17.50	BTKA
ATOM	1384	CA	MET	570	9.629	31.528	19.769	1.00	16.12	BTKA
ATOM	1385	CB	MET	570	8.588	32.073	18.797	1.00	16.10	BTKA
ATOM	1386	CG	MET	570	8.490	33.593	18.830	1.00	17.26	BTKA

	Atom Number	Atom Type	Amino Acid Residue		X	Y	Z	Occ.	Temp Factor	
ATOM	1387	SD	MET	570	7.274	34.254	17.686	1.00	27.62	BTKA
ATOM	1388	CE	MET	570	8.296	34.747	16.354	1.00	23.00	BTKA
ATOM	1389	C	MET	570	9.404	30.043	20.028	1.00	12.94	BTKA
ATOM	1390	O	MET	570	8.637	29.689	20.923	1.00	15.56	BTKA
ATOM	1391	N	TYR	571	10.027	29.172	19.242	1.00	12.61	BTKA
ATOM	1392	CA	TYR	571	9.875	27.726	19.448	1.00	14.91	BTKA
ATOM	1393	CB	TYR	571	8.489	27.216	19.010	1.00	17.43	BTKA
ATOM	1394	CG	TYR	571	8.126	27.460	17.560	1.00	16.93	BTKA
ATOM	1395	CD1	TYR	571	7.914	26.397	16.691	1.00	17.22	BTKA
ATOM	1396	CE1	TYR	571	7.565	26.612	15.361	1.00	18.55	BTKA
ATOM	1397	CD2	TYR	571	7.983	28.754	17.067	1.00	15.52	BTKA
ATOM	1398	CE2	TYR	571	7.640	28.987	15.742	1.00	21.13	BTKA
ATOM	1399	CZ	TYR	571	7.428	27.912	14.891	1.00	22.58	BTKA
ATOM	1400	OH	TYR	571	7.070	28.139	13.582	1.00	18.95	BTKA
ATOM	1401	C	TYR	571	10.983	26.881	18.832	1.00	15.24	BTKA
ATOM	1402	O	TYR	571	10.734	25.810	18.286	1.00	17.04	BTKA
ATOM	1403	N	SER	572	12.204	27.398	18.894	1.00	19.07	BTKA
ATOM	1404	CA	SER	572	13.383	26.696	18.399	1.00	19.19	BTKA
ATOM	1405	CB	SER	572	13.759	25.611	19.399	1.00	16.09	BTKA
ATOM	1406	OG	SER	572	13.662	26.109	20.727	1.00	13.53	BTKA
ATOM	1407	C	SER	572	13.270	26.088	17.001	1.00	19.87	BTKA
ATOM	1408	O	SER	572	13.729	24.960	16.761	1.00	16.73	BTKA
ATOM	1409	N	LYS	573	12.679	26.838	16.076	1.00	22.09	BTKA
ATOM	1410	CA	LYS	573	12.535	26.364	14.707	1.00	23.82	BTKA
ATOM	1411	CB	LYS	573	11.304	27.005	14.060	1.00	24.62	BTKA
ATOM	1412	CG	LYS	573	10.870	26.369	12.755	1.00	24.09	BTKA
ATOM	1413	CD	LYS	573	9.561	26.969	12.289	1.00	27.34	BTKA
ATOM	1414	CE	LYS	573	8.914	26.145	11.197	1.00	27.52	BTKA
ATOM	1415	NZ	LYS	573	7.495	26.549	11.009	1.00	27.13	BTKA
ATOM	1416	C	LYS	573	13.810	26.672	13.898	1.00	24.62	BTKA
ATOM	1417	O	LYS	573	13.875	27.661	13.159	1.00	24.59	BTKA
ATOM	1418	N	PHE	574	14.842	25.857	14.093	1.00	21.87	BTKA
ATOM	1419	CA	PHE	574	16.096	26.042	13.379	1.00	17.67	BTKA
ATOM	1420	CB	PHE	574	17.238	25.268	14.055	1.00	18.29	BTKA
ATOM	1421	CG	PHE	574	17.489	25.649	15.493	1.00	17.48	BTKA
ATOM	1422	CD1	PHE	574	17.065	24.823	16.527	1.00	20.56	BTKA
ATOM	1423	CD2	PHE	574	18.200	26.803	15.813	1.00	19.16	BTKA
ATOM	1424	CE1	PHE	574	17.345	25.132	17.860	1.00	20.84	BTKA
ATOM	1425	CE2	PHE	574	18.485	27.122	17.144	1.00	19.40	BTKA
ATOM	1426	CZ	PHE	574	18.054	26.280	18.168	1.00	17.92	BTKA
ATOM	1427	C	PHE	574	15.941	25.514	11.960	1.00	13.16	BTKA
ATOM	1428	O	PHE	574	15.181	24.577	11.716	1.00	13.27	BTKA
ATOM	1429	N	SER	575	16.668	26.112	11.028	1.00	13.22	BTKA
ATOM	1430	CA	SER	575	16.658	25.682	9.634	1.00	12.31	BTKA
ATOM	1431	CB	SER	575	15.405	26.185	8.900	1.00	9.44	BTKA
ATOM	1432	OG	SER	575	15.558	27.510	8.406	1.00	5.32	BTKA
ATOM	1433	C	SER	575	17.915	26.275	9.017	1.00	13.34	BTKA
ATOM	1434	O	SER	575	18.848	26.636	9.738	1.00	16.79	BTKA
ATOM	1435	N	SER	576	17.953	26.378	7.696	1.00	12.36	BTKA
ATOM	1436	CA	SER	576	19.102	26.959	7.033	1.00	11.50	BTKA
ATOM	1437	CB	SER	576	19.033	26.673	5.534	1.00	17.69	BTKA
ATOM	1438	OG	SER	576	17.829	27.186	4.970	1.00	25.45	BTKA
ATOM	1439	C	SER	576	19.048	28.465	7.250	1.00	9.00	BTKA
ATOM	1440	O	SER	576	20.068	29.129	7.436	1.00	11.10	BTKA
ATOM	1441	N	LYS	577	17.833	28.995	7.247	1.00	9.50	BTKA
ATOM	1442	CA	LYS	577	17.604	30.422	7.402	1.00	9.17	BTKA
ATOM	1443	CB	LYS	577	16.190	30.765	6.925	1.00	12.09	BTKA
ATOM	1444	CG	LYS	577	15.892	30.249	5.508	1.00	8.29	BTKA

Atom Number	Atom Type	Amino Acid Residue		X	Y	Z	Occ.	Temp Factor	
ATOM 1445	CD	LYS	577	16.752	30.956	4.471	1.00	19.55	BTKA
ATOM 1446	CE	LYS	577	16.830	30.179	3.159	1.00	15.68	BTKA
ATOM 1447	NZ	LYS	577	15.498	29.738	2.670	1.00	20.19	BTKA
ATOM 1448	C	LYS	577	17.878	30.940	8.812	1.00	8.67	BTKA
ATOM 1449	O	LYS	577	17.909	32.154	9.032	1.00	9.38	BTKA
ATOM 1450	N	SER	578	18.054	30.026	9.766	1.00	10.63	BTKA
ATOM 1451	CA	SER	578	18.378	30.401	11.141	1.00	7.64	BTKA
ATOM 1452	CB	SER	578	18.107	29.250	12.110	1.00	6.86	BTKA
ATOM 1453	OG	SER	578	16.743	28.879	12.106	1.00	18.48	BTKA
ATOM 1454	C	SER	578	19.862	30.743	11.139	1.00	3.05	BTKA
ATOM 1455	O	SER	578	20.281	31.699	11.785	1.00	3.62	BTKA
ATOM 1456	N	ASP	579	20.653	29.951	10.415	1.00	4.90	BTKA
ATOM 1457	CA	ASP	579	22.092	30.205	10.277	1.00	7.88	BTKA
ATOM 1458	CB	ASP	579	22.773	29.075	9.522	1.00	7.80	BTKA
ATOM 1459	CG	ASP	579	22.916	27.838	10.341	1.00	13.43	BTKA
ATOM 1460	OD1	ASP	579	22.190	27.698	11.347	1.00	16.68	BTKA
ATOM 1461	OD2	ASP	579	23.765	27.003	9.970	1.00	17.47	BTKA
ATOM 1462	C	ASP	579	22.330	31.496	9.500	1.00	5.97	BTKA
ATOM 1463	O	ASP	579	23.275	32.228	9.776	1.00	6.23	BTKA
ATOM 1464	N	ILE	580	21.515	31.715	8.472	1.00	6.76	BTKA
ATOM 1465	CA	ILE	580	21.607	32.921	7.652	1.00	8.95	BTKA
ATOM 1466	CB	ILE	580	20.548	32.921	6.497	1.00	7.78	BTKA
ATOM 1467	CG2	ILE	580	19.670	34.171	6.529	1.00	9.49	BTKA
ATOM 1468	CG1	ILE	580	21.252	32.861	5.136	1.00	6.38	BTKA
ATOM 1469	CD	ILE	580	21.449	31.477	4.617	1.00	12.06	BTKA
ATOM 1470	C	ILE	580	21.452	34.150	8.545	1.00	9.29	BTKA
ATOM 1471	O	ILE	580	22.247	35.087	8.449	1.00	14.35	BTKA
ATOM 1472	N	TRP	581	20.457	34.127	9.430	1.00	8.74	BTKA
ATOM 1473	CA	TRP	581	20.218	35.235	10.339	1.00	4.45	BTKA
ATOM 1474	CB	TRP	581	18.997	34.961	11.219	1.00	5.26	BTKA
ATOM 1475	CG	TRP	581	18.656	36.080	12.187	1.00	5.57	BTKA
ATOM 1476	CD2	TRP	581	17.478	36.894	12.182	1.00	7.10	BTKA
ATOM 1477	CE2	TRP	581	17.577	37.782	13.276	1.00	8.85	BTKA
ATOM 1478	CE3	TRP	581	16.343	36.957	11.366	1.00	5.60	BTKA
ATOM 1479	CD1	TRP	581	19.400	36.500	13.253	1.00	7.88	BTKA
ATOM 1480	NE1	TRP	581	18.760	37.520	13.908	1.00	8.39	BTKA
ATOM 1481	CZ2	TRP	581	16.590	38.716	13.571	1.00	7.26	BTKA
ATOM 1482	CZ3	TRP	581	15.364	37.885	11.661	1.00	2.00	BTKA
ATOM 1483	CH2	TRP	581	15.495	38.752	12.753	1.00	6.05	BTKA
ATOM 1484	C	TRP	581	21.442	35.446	11.195	1.00	4.23	BTKA
ATOM 1485	O	TRP	581	21.953	36.557	11.290	1.00	7.98	BTKA
ATOM 1486	N	ALA	582	21.907	34.371	11.821	1.00	9.71	BTKA
ATOM 1487	CA	ALA	582	23.083	34.408	12.690	1.00	7.74	BTKA
ATOM 1488	CB	ALA	582	23.304	33.041	13.314	1.00	5.41	BTKA
ATOM 1489	C	ALA	582	24.342	34.878	11.957	1.00	9.07	BTKA
ATOM 1490	O	ALA	582	25.189	35.551	12.543	1.00	8.09	BTKA
ATOM 1491	N	PHE	583	24.463	34.522	10.675	1.00	12.09	BTKA
ATOM 1492	CA	PHE	583	25.609	34.920	9.841	1.00	7.60	BTKA
ATOM 1493	CB	PHE	583	25.557	34.201	8.490	1.00	9.22	BTKA
ATOM 1494	CG	PHE	583	26.526	34.740	7.465	1.00	4.47	BTKA
ATOM 1495	CD1	PHE	583	27.877	34.430	7.536	1.00	4.68	BTKA
ATOM 1496	CD2	PHE	583	26.079	35.549	6.421	1.00	6.35	BTKA
ATOM 1497	CE1	PHE	583	28.769	34.915	6.585	1.00	5.23	BTKA
ATOM 1498	CE2	PHE	583	26.969	36.039	5.460	1.00	2.15	BTKA
ATOM 1499	CZ	PHE	583	28.313	35.719	5.545	1.00	5.61	BTKA
ATOM 1500	C	PHE	583	25.536	36.416	9.607	1.00	10.14	BTKA
ATOM 1501	O	PHE	583	26.556	37.111	9.615	1.00	11.69	BTKA
ATOM 1502	N	GLY	584	24.320	36.895	9.360	1.00	10.66	BTKA

Atom Number	Atom Type	Amino Acid Residue		X	Y	Z	Occ.	Temp Factor	
ATOM	1503	CA	GLY 584	24.102	38.309	9.128	1.00	9.30	BTKA
ATOM	1504	C	GLY 584	24.514	39.107	10.339	1.00	7.76	BTKA
ATOM	1505	O	GLY 584	25.051	40.209	10.212	1.00	10.68	BTKA
ATOM	1506	N	VAL 585	24.259	38.559	11.525	1.00	7.75	BTKA
ATOM	1507	CA	VAL 585	24.644	39.246	12.750	1.00	6.19	BTKA
ATOM	1508	CB	VAL 585	23.995	38.628	14.015	1.00	5.76	BTKA
ATOM	1509	CG1	VAL 585	24.471	39.358	15.246	1.00	8.91	BTKA
ATOM	1510	CG2	VAL 585	22.478	38.711	13.945	1.00	4.10	BTKA
ATOM	1511	C	VAL 585	26.169	39.169	12.847	1.00	7.35	BTKA
ATOM	1512	O	VAL 585	26.818	40.145	13.201	1.00	10.25	BTKA
ATOM	1513	N	LEU 586	26.746	38.026	12.487	1.00	4.16	BTKA
ATOM	1514	CA	LEU 586	28.200	37.873	12.527	1.00	7.72	BTKA
ATOM	1515	CB	LEU 586	28.632	36.492	12.005	1.00	5.58	BTKA
ATOM	1516	CG	LEU 586	30.127	36.293	11.693	1.00	6.32	BTKA
ATOM	1517	CD1	LEU 586	31.005	36.643	12.885	1.00	2.00	BTKA
ATOM	1518	CD2	LEU 586	30.385	34.880	11.254	1.00	6.90	BTKA
ATOM	1519	C	LEU 586	28.857	38.965	11.695	1.00	6.55	BTKA
ATOM	1520	O	LEU 586	29.902	39.502	12.071	1.00	6.94	BTKA
ATOM	1521	N	MET 587	28.242	39.278	10.557	1.00	9.63	BTKA
ATOM	1522	CA	MET 587	28.745	40.310	9.660	1.00	5.25	BTKA
ATOM	1523	CB	MET 587	27.850	40.442	8.437	1.00	5.01	BTKA
ATOM	1524	CG	MET 587	27.974	39.317	7.443	1.00	4.97	BTKA
ATOM	1525	SD	MET 587	27.187	39.797	5.910	1.00	9.68	BTKA
ATOM	1526	CE	MET 587	28.480	40.808	5.189	1.00	3.35	BTKA
ATOM	1527	C	MET 587	28.755	41.626	10.400	1.00	6.90	BTKA
ATOM	1528	O	MET 587	29.716	42.387	10.318	1.00	4.22	BTKA
ATOM	1529	N	TRP 588	27.680	41.878	11.143	1.00	8.72	BTKA
ATOM	1530	CA	TRP 588	27.551	43.096	11.925	1.00	9.02	BTKA
ATOM	1531	CB	TRP 588	26.176	43.155	12.595	1.00	7.30	BTKA
ATOM	1532	CG	TRP 588	25.977	44.397	13.389	1.00	3.41	BTKA
ATOM	1533	CD2	TRP 588	26.321	44.593	14.759	1.00	5.76	BTKA
ATOM	1534	CE2	TRP 588	26.021	45.939	15.078	1.00	3.37	BTKA
ATOM	1535	CE3	TRP 588	26.863	43.765	15.756	1.00	7.65	BTKA
ATOM	1536	CD1	TRP 588	25.492	45.591	12.941	1.00	3.84	BTKA
ATOM	1537	NE1	TRP 588	25.518	46.525	13.946	1.00	2.00	BTKA
ATOM	1538	CZ2	TRP 588	26.244	46.470	16.348	1.00	3.23	BTKA
ATOM	1539	CZ3	TRP 588	27.085	44.298	17.012	1.00	2.00	BTKA
ATOM	1540	CH2	TRP 588	26.777	45.635	17.298	1.00	5.01	BTKA
ATOM	1541	C	TRP 588	28.655	43.122	12.980	1.00	11.28	BTKA
ATOM	1542	O	TRP 588	29.133	44.186	13.362	1.00	11.93	BTKA
ATOM	1543	N	GLU 589	29.058	41.942	13.439	1.00	11.46	BTKA
ATOM	1544	CA	GLU 589	30.116	41.828	14.430	1.00	10.29	BTKA
ATOM	1545	CB	GLU 589	30.177	40.409	15.010	1.00	10.54	BTKA
ATOM	1546	CG	GLU 589	28.996	40.024	15.873	1.00	6.40	BTKA
ATOM	1547	CD	GLU 589	29.184	38.674	16.522	1.00	5.99	BTKA
ATOM	1548	OE1	GLU 589	29.688	38.628	17.661	1.00	10.51	BTKA
ATOM	1549	OE2	GLU 589	28.835	37.654	15.890	1.00	5.23	BTKA
ATOM	1550	C	GLU 589	31.442	42.164	13.768	1.00	11.38	BTKA
ATOM	1551	O	GLU 589	32.287	42.844	14.349	1.00	9.66	BTKA
ATOM	1552	N	ILE 590	31.632	41.666	12.554	1.00	9.79	BTKA
ATOM	1553	CA	ILE 590	32.860	41.931	11.825	1.00	14.53	BTKA
ATOM	1554	CB	ILE 590	32.921	41.136	10.476	1.00	13.48	BTKA
ATOM	1555	CG2	ILE 590	34.080	41.612	9.628	1.00	13.14	BTKA
ATOM	1556	CG1	ILE 590	33.080	39.637	10.746	1.00	14.32	BTKA
ATOM	1557	CD	ILE 590	33.136	38.788	9.489	1.00	2.34	BTKA
ATOM	1558	C	ILE 590	32.982	43.426	11.552	1.00	14.06	BTKA
ATOM	1559	O	ILE 590	33.983	44.052	11.908	1.00	15.05	BTKA
ATOM	1560	N	TYR 591	31.931	44.007	10.982	1.00	14.63	BTKA

	Atom Number	Atom Type	Amino Acid Residue		X	Y	Z	Occ.	Temp Factor	
ATOM	1561	CA	TYR	591	31.939	45.423	10.642	1.00	10.81	BTKA
ATOM	1562	CB	TYR	591	30.878	45.721	9.592	1.00	11.09	BTKA
ATOM	1563	CG	TYR	591	31.410	45.434	8.213	1.00	11.87	BTKA
ATOM	1564	CD1	TYR	591	31.381	44.144	7.684	1.00	15.61	BTKA
ATOM	1565	CE1	TYR	591	31.955	43.863	6.446	1.00	11.16	BTKA
ATOM	1566	CD2	TYR	591	32.022	46.437	7.466	1.00	10.34	BTKA
ATOM	1567	CE2	TYR	591	32.598	46.170	6.235	1.00	10.30	BTKA
ATOM	1568	CZ	TYR	591	32.564	44.883	5.731	1.00	11.77	BTKA
ATOM	1569	OH	TYR	591	33.154	44.620	4.519	1.00	18.27	BTKA
ATOM	1570	C	TYR	591	31.964	46.440	11.780	1.00	8.81	BTKA
ATOM	1571	O	TYR	591	32.575	47.505	11.645	1.00	9.70	BTKA
ATOM	1572	N	SER	592	31.330	46.126	12.904	1.00	9.16	BTKA
ATOM	1573	CA	SER	592	31.377	47.033	14.051	1.00	10.14	BTKA
ATOM	1574	CB	SER	592	30.157	46.849	14.961	1.00	8.60	BTKA
ATOM	1575	OG	SER	592	30.143	45.577	15.572	1.00	10.12	BTKA
ATOM	1576	C	SER	592	32.684	46.776	14.823	1.00	11.91	BTKA
ATOM	1577	O	SER	592	32.904	47.341	15.894	1.00	12.09	BTKA
ATOM	1578	N	LEU	593	33.554	45.944	14.247	1.00	8.44	BTKA
ATOM	1579	CA	LEU	593	34.837	45.583	14.836	1.00	11.62	BTKA
ATOM	1580	CB	LEU	593	35.794	46.784	14.878	1.00	11.72	BTKA
ATOM	1581	CG	LEU	593	36.273	47.296	13.507	1.00	13.96	BTKA
ATOM	1582	CD1	LEU	593	37.035	48.602	13.641	1.00	11.23	BTKA
ATOM	1583	CD2	LEU	593	37.130	46.246	12.820	1.00	13.30	BTKA
ATOM	1584	C	LEU	593	34.757	44.901	16.197	1.00	13.49	BTKA
ATOM	1585	O	LEU	593	35.398	45.324	17.158	1.00	15.34	BTKA
ATOM	1586	N	GLY	594	33.984	43.820	16.249	1.00	13.34	BTKA
ATOM	1587	CA	GLY	594	33.842	43.027	17.460	1.00	13.43	BTKA
ATOM	1588	C	GLY	594	32.899	43.478	18.554	1.00	12.35	BTKA
ATOM	1589	O	GLY	594	33.053	43.074	19.702	1.00	16.26	BTKA
ATOM	1590	N	LYS	595	31.907	44.292	18.225	1.00	15.44	BTKA
ATOM	1591	CA	LYS	595	30.982	44.751	19.252	1.00	14.58	BTKA
ATOM	1592	CB	LYS	595	30.422	46.133	18.902	1.00	16.29	BTKA
ATOM	1593	CG	LYS	595	31.498	47.153	18.538	1.00	17.65	BTKA
ATOM	1594	CD	LYS	595	32.699	47.035	19.468	1.00	20.70	BTKA
ATOM	1595	CE	LYS	595	33.937	47.733	18.911	1.00	19.00	BTKA
ATOM	1596	NZ	LYS	595	35.142	47.357	19.707	1.00	21.27	BTKA
ATOM	1597	C	LYS	595	29.862	43.746	19.481	1.00	11.31	BTKA
ATOM	1598	O	LYS	595	29.561	42.941	18.600	1.00	11.64	BTKA
ATOM	1599	N	MET	596	29.311	43.743	20.695	1.00	13.47	BTKA
ATOM	1600	CA	MET	596	28.212	42.842	21.044	1.00	13.02	BTKA
ATOM	1601	CB	MET	596	28.097	42.639	22.569	1.00	17.06	BTKA
ATOM	1602	CG	MET	596	26.706	42.143	23.017	1.00	18.96	BTKA
ATOM	1603	SD	MET	596	26.594	41.087	24.493	1.00	25.10	BTKA
ATOM	1604	CE	MET	596	26.050	42.271	25.755	1.00	16.77	BTKA
ATOM	1605	C	MET	596	26.908	43.396	20.502	1.00	8.51	BTKA
ATOM	1606	O	MET	596	26.670	44.611	20.547	1.00	8.39	BTKA
ATOM	1607	N	PRO	597	26.042	42.511	19.986	1.00	6.79	BTKA
ATOM	1608	CD	PRO	597	26.280	41.091	19.679	1.00	2.92	BTKA
ATOM	1609	CA	PRO	597	24.760	42.938	19.441	1.00	7.77	BTKA
ATOM	1610	CB	PRO	597	24.283	41.694	18.679	1.00	2.29	BTKA
ATOM	1611	CG	PRO	597	25.559	40.945	18.387	1.00	2.89	BTKA
ATOM	1612	C	PRO	597	23.791	43.330	20.541	1.00	5.87	BTKA
ATOM	1613	O	PRO	597	23.608	42.598	21.504	1.00	8.10	BTKA
ATOM	1614	N	TYR	598	23.198	44.509	20.421	1.00	11.67	BTKA
ATOM	1615	CA	TYR	598	22.225	44.984	21.403	1.00	11.39	BTKA
ATOM	1616	CB	TYR	598	20.986	44.087	21.374	1.00	11.13	BTKA
ATOM	1617	CG	TYR	598	20.502	43.671	20.010	1.00	10.46	BTKA
ATOM	1618	CD1	TYR	598	20.737	42.384	19.538	1.00	8.57	BTKA

Atom Number	Atom Type	Amino Acid Residue		X	Y	Z	Occ.	Temp Factor	
ATOM	1619	CE1	TYR 598	20.241	41.968	18.321	1.00	9.01	BTKA
ATOM	1620	CD2	TYR 598	19.757	44.541	19.219	1.00	11.82	BTKA
ATOM	1621	CE2	TYR 598	19.255	44.139	17.998	1.00	11.15	BTKA
ATOM	1622	CZ	TYR 598	19.499	42.850	17.553	1.00	10.70	BTKA
ATOM	1623	OH	TYR 598	19.007	42.443	16.335	1.00	12.06	BTKA
ATOM	1624	C	TYR 598	22.731	45.018	22.851	1.00	13.88	BTKA
ATOM	1625	O	TYR 598	21.993	44.656	23.762	1.00	14.96	BTKA
ATOM	1626	N	GLU 599	23.940	45.518	23.078	1.00	17.51	BTKA
ATOM	1627	CA	GLU 599	24.506	45.556	24.434	1.00	21.90	BTKA
ATOM	1628	CB	GLU 599	25.965	46.063	24.418	1.00	25.83	BTKA
ATOM	1629	CG	GLU 599	26.155	47.580	24.303	1.00	25.70	BTKA
ATOM	1630	CD	GLU 599	25.989	48.100	22.887	1.00	29.61	BTKA
ATOM	1631	OE1	GLU 599	24.842	48.148	22.385	1.00	34.92	BTKA
ATOM	1632	OE2	GLU 599	27.018	48.465	22.275	1.00	36.19	BTKA
ATOM	1633	C	GLU 599	23.707	46.290	25.523	1.00	22.83	BTKA
ATOM	1634	O	GLU 599	23.867	45.990	26.704	1.00	21.63	BTKA
ATOM	1635	N	ARG 600	22.903	47.285	25.157	1.00	23.83	BTKA
ATOM	1636	CA	ARG 600	22.120	47.991	26.170	1.00	25.44	BTKA
ATOM	1637	CB	ARG 600	21.977	49.477	25.857	1.00	23.52	BTKA
ATOM	1638	CG	ARG 600	22.569	50.385	26.941	1.00	27.22	BTKA
ATOM	1639	CD	ARG 600	21.939	50.168	28.326	1.00	31.56	BTKA
ATOM	1640	NE	ARG 600	22.425	51.152	29.296	1.00	30.45	BTKA
ATOM	1641	CZ	ARG 600	21.656	51.847	30.136	1.00	28.69	BTKA
ATOM	1642	NH1	ARG 600	22.211	52.726	30.960	1.00	27.63	BTKA
ATOM	1643	NH2	ARG 600	20.344	51.659	30.175	1.00	26.46	BTKA
ATOM	1644	C	ARG 600	20.750	47.351	26.356	1.00	26.74	BTKA
ATOM	1645	O	ARG 600	19.931	47.818	27.162	1.00	27.64	BTKA
ATOM	1646	N	PHE 601	20.492	46.309	25.571	1.00	24.54	BTKA
ATOM	1647	CA	PHE 601	19.243	45.573	25.664	1.00	20.59	BTKA
ATOM	1648	CB	PHE 601	18.841	44.989	24.305	1.00	22.31	BTKA
ATOM	1649	CG	PHE 601	18.485	46.006	23.266	1.00	22.63	BTKA
ATOM	1650	CD1	PHE 601	17.177	46.128	22.823	1.00	23.34	BTKA
ATOM	1651	CD2	PHE 601	19.460	46.791	22.677	1.00	20.08	BTKA
ATOM	1652	CE1	PHE 601	16.852	47.011	21.809	1.00	20.90	BTKA
ATOM	1653	CE2	PHE 601	19.138	47.674	21.660	1.00	20.46	BTKA
ATOM	1654	CZ	PHE 601	17.832	47.783	21.225	1.00	22.29	BTKA
ATOM	1655	C	PHE 601	19.511	44.399	26.588	1.00	20.01	BTKA
ATOM	1656	O	PHE 601	20.624	44.202	27.074	1.00	18.72	BTKA
ATOM	1657	N	THR 602	18.481	43.601	26.801	1.00	22.29	BTKA
ATOM	1658	CA	THR 602	18.582	42.400	27.604	1.00	23.72	BTKA
ATOM	1659	CB	THR 602	17.681	42.486	28.861	1.00	24.01	BTKA
ATOM	1660	OG1	THR 602	16.339	42.823	28.478	1.00	20.42	BTKA
ATOM	1661	CG2	THR 602	18.204	43.538	29.823	1.00	27.75	BTKA
ATOM	1662	C	THR 602	18.061	41.323	26.652	1.00	25.22	BTKA
ATOM	1663	O	THR 602	17.420	41.645	25.644	1.00	27.52	BTKA
ATOM	1664	N	ASN 603	18.333	40.055	26.939	1.00	26.65	BTKA
ATOM	1665	CA	ASN 603	17.844	38.979	26.072	1.00	25.54	BTKA
ATOM	1666	CB	ASN 603	18.192	37.607	26.662	1.00	20.91	BTKA
ATOM	1667	CG	ASN 603	19.674	37.298	26.576	1.00	25.12	BTKA
ATOM	1668	OD1	ASN 603	20.490	38.194	26.385	1.00	25.37	BTKA
ATOM	1669	ND2	ASN 603	20.026	36.028	26.704	1.00	26.15	BTKA
ATOM	1670	C	ASN 603	16.337	39.082	25.803	1.00	25.43	BTKA
ATOM	1671	O	ASN 603	15.864	38.698	24.736	1.00	23.83	BTKA
ATOM	1672	N	SER 604	15.597	39.655	26.747	1.00	26.48	BTKA
ATOM	1673	CA	SER 604	14.152	39.806	26.602	1.00	24.32	BTKA
ATOM	1674	CB	SER 604	13.487	39.881	27.977	1.00	24.89	BTKA
ATOM	1675	OG	SER 604	14.121	40.858	28.786	1.00	27.86	BTKA
ATOM	1676	C	SER 604	13.767	41.025	25.768	1.00	21.82	BTKA

	Atom Number	Atom Type	Amino Acid Residue		X	Y	Z	Occ.	Temp Factor	
ATOM	1677	O	SER	604	12.799	40.983	25.005	1.00	19.52	BTKA
ATOM	1678	N	GLU	605	14.505	42.118	25.933	1.00	23.74	BTKA
ATOM	1679	CA	GLU	605	14.229	43.343	25.181	1.00	21.76	BTKA
ATOM	1680	CB	GLU	605	14.937	44.543	25.815	1.00	19.06	BTKA
ATOM	1681	CG	GLU	605	14.413	44.880	27.213	1.00	21.14	BTKA
ATOM	1682	CD	GLU	605	15.253	45.914	27.930	1.00	18.46	BTKA
ATOM	1683	OE1	GLU	605	14.730	46.576	28.850	1.00	22.19	BTKA
ATOM	1684	OE2	GLU	605	16.443	46.064	27.583	1.00	25.21	BTKA
ATOM	1685	C	GLU	605	14.656	43.159	23.733	1.00	19.22	BTKA
ATOM	1686	O	GLU	605	14.020	43.688	22.820	1.00	17.88	BTKA
ATOM	1687	N	THR	606	15.710	42.374	23.534	1.00	19.68	BTKA
ATOM	1688	CA	THR	606	16.231	42.064	22.205	1.00	17.05	BTKA
ATOM	1689	CB	THR	606	17.471	41.148	22.306	1.00	15.00	BTKA
ATOM	1690	OG1	THR	606	18.458	41.769	23.139	1.00	15.89	BTKA
ATOM	1691	CG2	THR	606	18.056	40.871	20.938	1.00	12.52	BTKA
ATOM	1692	C	THR	606	15.138	41.339	21.418	1.00	16.80	BTKA
ATOM	1693	O	THR	606	14.900	41.637	20.243	1.00	18.76	BTKA
ATOM	1694	N	ALA	607	14.457	40.408	22.084	1.00	16.21	BTKA
ATOM	1695	CA	ALA	607	13.377	39.648	21.467	1.00	16.69	BTKA
ATOM	1696	CB	ALA	607	12.926	38.532	22.384	1.00	14.32	BTKA
ATOM	1697	C	ALA	607	12.211	40.573	21.138	1.00	17.62	BTKA
ATOM	1698	O	ALA	607	11.574	40.417	20.098	1.00	21.64	BTKA
ATOM	1699	N	GLU	608	11.940	41.540	22.015	1.00	16.80	BTKA
ATOM	1700	CA	GLU	608	10.855	42.497	21.792	1.00	17.47	BTKA
ATOM	1701	CB	GLU	608	10.574	43.312	23.064	1.00	24.26	BTKA
ATOM	1702	CG	GLU	608	9.979	42.503	24.219	1.00	31.87	BTKA
ATOM	1703	CD	GLU	608	9.562	43.363	25.414	1.00	32.17	BTKA
ATOM	1704	OE1	GLU	608	8.411	43.210	25.892	1.00	33.50	BTKA
ATOM	1705	OE2	GLU	608	10.386	44.183	25.886	1.00	34.89	BTKA
ATOM	1706	C	GLU	608	11.207	43.438	20.631	1.00	13.51	BTKA
ATOM	1707	O	GLU	608	10.370	43.714	19.765	1.00	5.86	BTKA
ATOM	1708	N	HIS	609	12.472	43.865	20.603	1.00	9.80	BTKA
ATOM	1709	CA	HIS	609	13.025	44.762	19.586	1.00	6.26	BTKA
ATOM	1710	CB	HIS	609	14.509	45.014	19.886	1.00	6.17	BTKA
ATOM	1711	CG	HIS	609	15.179	45.976	18.950	1.00	7.14	BTKA
ATOM	1712	CD2	HIS	609	15.978	45.769	17.879	1.00	9.08	BTKA
ATOM	1713	ND1	HIS	609	15.114	47.342	19.116	1.00	10.07	BTKA
ATOM	1714	CE1	HIS	609	15.848	47.935	18.192	1.00	4.17	BTKA
ATOM	1715	NE2	HIS	609	16.384	47.002	17.427	1.00	8.56	BTKA
ATOM	1716	C	HIS	609	12.881	44.121	18.221	1.00	9.48	BTKA
ATOM	1717	O	HIS	609	12.489	44.782	17.255	1.00	11.18	BTKA
ATOM	1718	N	ILE	610	13.214	42.839	18.138	1.00	8.84	BTKA
ATOM	1719	CA	ILE	610	13.106	42.113	16.881	1.00	11.99	BTKA
ATOM	1720	CB	ILE	610	13.869	40.758	16.945	1.00	13.75	BTKA
ATOM	1721	CG2	ILE	610	13.211	39.701	16.048	1.00	13.99	BTKA
ATOM	1722	CG1	ILE	610	15.345	40.991	16.594	1.00	6.66	BTKA
ATOM	1723	CD	ILE	610	16.188	39.734	16.592	1.00	8.43	BTKA
ATOM	1724	C	ILE	610	11.635	41.923	16.527	1.00	14.02	BTKA
ATOM	1725	O	ILE	610	11.257	41.964	15.356	1.00	12.60	BTKA
ATOM	1726	N	ALA	611	10.802	41.798	17.557	1.00	15.80	BTKA
ATOM	1727	CA	ALA	611	9.368	41.631	17.377	1.00	14.09	BTKA
ATOM	1728	CB	ALA	611	8.713	41.313	18.710	1.00	15.18	BTKA
ATOM	1729	C	ALA	611	8.759	42.889	16.767	1.00	13.18	BTKA
ATOM	1730	O	ALA	611	7.688	42.843	16.174	1.00	16.50	BTKA
ATOM	1731	N	GLN	612	9.448	44.012	16.918	1.00	9.26	BTKA
ATOM	1732	CA	GLN	612	8.996	45.288	16.369	1.00	9.32	BTKA
ATOM	1733	CB	GLN	612	9.538	46.438	17.214	1.00	12.00	BTKA
ATOM	1734	CG	GLN	612	9.266	46.315	18.699	1.00	15.05	BTKA

Atom	Number	Atom Type	Amino Acid Residue		X	Y	Z	Occ.	Temp Factor	
ATOM	1735	CD	GLN	612	8.041	47.065	19.115	1.00	19.92	BTKA
ATOM	1736	OE1	GLN	612	6.918	46.656	18.833	1.00	26.26	BTKA
ATOM	1737	NE2	GLN	612	8.246	48.194	19.773	1.00	24.14	BTKA
ATOM	1738	C	GLN	612	9.497	45.470	14.939	1.00	8.38	BTKA
ATOM	1739	O	GLN	612	9.184	46.471	14.285	1.00	8.92	BTKA
ATOM	1740	N	GLY	613	10.308	44.523	14.476	1.00	11.09	BTKA
ATOM	1741	CA	GLY	613	10.861	44.598	13.135	1.00	10.83	BTKA
ATOM	1742	C	GLY	613	12.164	45.381	13.076	1.00	12.46	BTKA
ATOM	1743	O	GLY	613	12.642	45.711	11.993	1.00	8.12	BTKA
ATOM	1744	N	LEU	614	12.736	45.690	14.237	1.00	10.93	BTKA
ATOM	1745	CA	LEU	614	13.988	46.439	14.300	1.00	11.92	BTKA
ATOM	1746	CB	LEU	614	14.012	47.375	15.518	1.00	9.21	BTKA
ATOM	1747	CG	LEU	614	13.103	48.609	15.581	1.00	11.29	BTKA
ATOM	1748	CD1	LEU	614	12.426	48.880	14.249	1.00	11.46	BTKA
ATOM	1749	CD2	LEU	614	12.078	48.433	16.656	1.00	4.88	BTKA
ATOM	1750	C	LEU	614	15.188	45.495	14.330	1.00	11.01	BTKA
ATOM	1751	O	LEU	614	15.148	44.424	14.947	1.00	9.79	BTKA
ATOM	1752	N	ARG	615	16.273	45.920	13.694	1.00	12.00	BTKA
ATOM	1753	CA	ARG	615	17.484	45.117	13.603	1.00	9.33	BTKA
ATOM	1754	CB	ARG	615	17.704	44.713	12.144	1.00	9.55	BTKA
ATOM	1755	CG	ARG	615	16.518	44.023	11.488	1.00	7.26	BTKA
ATOM	1756	CD	ARG	615	16.209	42.703	12.141	1.00	3.51	BTKA
ATOM	1757	NE	ARG	615	15.114	42.016	11.473	1.00	7.24	BTKA
ATOM	1758	CZ	ARG	615	13.889	41.891	11.976	1.00	8.86	BTKA
ATOM	1759	NH1	ARG	615	13.582	42.421	13.156	1.00	7.13	BTKA
ATOM	1760	NH2	ARG	615	12.986	41.170	11.329	1.00	8.16	BTKA
ATOM	1761	C	ARG	615	18.704	45.885	14.098	1.00	8.91	BTKA
ATOM	1762	O	ARG	615	18.570	46.921	14.762	1.00	7.60	BTKA
ATOM	1763	N	LEU	616	19.887	45.379	13.756	1.00	7.61	BTKA
ATOM	1764	CA	LEU	616	21.155	45.990	14.138	1.00	9.07	BTKA
ATOM	1765	CB	LEU	616	22.255	44.927	14.183	1.00	9.04	BTKA
ATOM	1766	CG	LEU	616	22.202	43.944	15.355	1.00	9.90	BTKA
ATOM	1767	CD1	LEU	616	23.034	42.705	15.046	1.00	6.52	BTKA
ATOM	1768	CD2	LEU	616	22.690	44.632	16.623	1.00	8.47	BTKA
ATOM	1769	C	LEU	616	21.545	47.094	13.162	1.00	7.88	BTKA
ATOM	1770	O	LEU	616	21.682	46.848	11.965	1.00	11.49	BTKA
ATOM	1771	N	TYR	617	21.770	48.295	13.696	1.00	9.86	BTKA
ATOM	1772	CA	TYR	617	22.133	49.480	12.913	1.00	6.95	BTKA
ATOM	1773	CB	TYR	617	22.440	50.653	13.853	1.00	8.23	BTKA
ATOM	1774	CG	TYR	617	23.719	50.515	14.674	1.00	11.82	BTKA
ATOM	1775	CD1	TYR	617	24.923	51.090	14.244	1.00	11.55	BTKA
ATOM	1776	CE1	TYR	617	26.086	51.011	15.021	1.00	9.18	BTKA
ATOM	1777	CD2	TYR	617	23.714	49.856	15.897	1.00	10.14	BTKA
ATOM	1778	CE2	TYR	617	24.869	49.777	16.682	1.00	15.29	BTKA
ATOM	1779	CZ	TYR	617	26.047	50.358	16.240	1.00	13.29	BTKA
ATOM	1780	OH	TYR	617	27.167	50.305	17.043	1.00	10.85	BTKA
ATOM	1781	C	TYR	617	23.315	49.298	11.962	1.00	7.09	BTKA
ATOM	1782	O	TYR	617	24.166	48.440	12.182	1.00	6.00	BTKA
ATOM	1783	N	ARG	618	23.391	50.146	10.938	1.00	7.06	BTKA
ATOM	1784	CA	ARG	618	24.498	50.072	9.990	1.00	13.07	BTKA
ATOM	1785	CB	ARG	618	24.271	50.947	8.752	1.00	11.95	BTKA
ATOM	1786	CG	ARG	618	25.389	50.761	7.721	1.00	12.02	BTKA
ATOM	1787	CD	ARG	618	25.823	52.046	7.028	1.00	12.70	BTKA
ATOM	1788	NE	ARG	618	24.896	52.504	5.996	1.00	10.05	BTKA
ATOM	1789	CZ	ARG	618	25.263	53.226	4.939	1.00	8.38	BTKA
ATOM	1790	NH1	ARG	618	26.535	53.561	4.769	1.00	8.75	BTKA
ATOM	1791	NH2	ARG	618	24.352	53.659	4.076	1.00	8.27	BTKA
ATOM	1792	C	ARG	618	25.767	50.547	10.668	1.00	15.11	BTKA

Atom	Number	Atom Type	Amino Acid Residue		X	Y	Z	Occ.	Temp Factor	
ATOM	1793	O	ARG	618	25.798	51.647	11.223	1.00	18.30	BTKA
ATOM	1794	N	PRO	619	26.803	49.694	10.713	1.00	17.30	BTKA
ATOM	1795	CD	PRO	619	26.790	48.234	10.509	1.00	15.23	BTKA
ATOM	1796	CA	PRO	619	28.045	50.130	11.353	1.00	16.98	BTKA
ATOM	1797	CB	PRO	619	28.740	48.808	11.683	1.00	16.78	BTKA
ATOM	1798	CG	PRO	619	28.237	47.876	10.651	1.00	13.87	BTKA
ATOM	1799	C	PRO	619	28.871	51.039	10.430	1.00	16.87	BTKA
ATOM	1800	O	PRO	619	28.956	50.805	9.229	1.00	15.47	BTKA
ATOM	1801	N	HIS	620	29.429	52.101	11.008	1.00	16.43	BTKA
ATOM	1802	CA	HIS	620	30.243	53.088	10.287	1.00	19.75	BTKA
ATOM	1803	CB	HIS	620	30.946	54.021	11.290	1.00	19.36	BTKA
ATOM	1804	CG	HIS	620	31.863	53.317	12.247	1.00	20.09	BTKA
ATOM	1805	CD2	HIS	620	33.211	53.355	12.384	1.00	21.52	BTKA
ATOM	1806	ND1	HIS	620	31.407	52.455	13.222	1.00	20.76	BTKA
ATOM	1807	CE1	HIS	620	32.434	51.988	13.912	1.00	16.73	BTKA
ATOM	1808	NE2	HIS	620	33.538	52.519	13.423	1.00	17.10	BTKA
ATOM	1809	C	HIS	620	31.257	52.589	9.239	1.00	21.42	BTKA
ATOM	1810	O	HIS	620	31.646	53.344	8.347	1.00	22.39	BTKA
ATOM	1811	N	LEU	621	31.695	51.338	9.346	1.00	19.75	BTKA
ATOM	1812	CA	LEU	621	32.661	50.793	8.396	1.00	16.60	BTKA
ATOM	1813	CB	LEU	621	33.712	49.948	9.118	1.00	13.75	BTKA
ATOM	1814	CG	LEU	621	34.539	50.612	10.226	1.00	9.81	BTKA
ATOM	1815	CD1	LEU	621	35.542	49.613	10.742	1.00	4.63	BTKA
ATOM	1816	CD2	LEU	621	35.248	51.863	9.713	1.00	9.43	BTKA
ATOM	1817	C	LEU	621	32.010	49.966	7.296	1.00	17.19	BTKA
ATOM	1818	O	LEU	621	32.694	49.260	6.558	1.00	18.71	BTKA
ATOM	1819	N	ALA	622	30.690	50.054	7.184	1.00	18.73	BTKA
ATOM	1820	CA	ALA	622	29.958	49.309	6.171	1.00	14.75	BTKA
ATOM	1821	CB	ALA	622	28.886	48.449	6.826	1.00	16.96	BTKA
ATOM	1822	C	ALA	622	29.322	50.248	5.158	1.00	14.61	BTKA
ATOM	1823	O	ALA	622	28.808	51.309	5.512	1.00	15.18	BTKA
ATOM	1824	N	SER	623	29.396	49.875	3.886	1.00	16.92	BTKA
ATOM	1825	CA	SER	623	28.793	50.670	2.825	1.00	14.96	BTKA
ATOM	1826	CB	SER	623	29.433	50.326	1.479	1.00	10.06	BTKA
ATOM	1827	OG	SER	623	29.253	48.958	1.163	1.00	7.67	BTKA
ATOM	1828	C	SER	623	27.309	50.336	2.785	1.00	13.91	BTKA
ATOM	1829	O	SER	623	26.867	49.392	3.433	1.00	15.97	BTKA
ATOM	1830	N	GLU	624	26.541	51.112	2.028	1.00	15.15	BTKA
ATOM	1831	CA	GLU	624	25.110	50.868	1.888	1.00	16.38	BTKA
ATOM	1832	CB	GLU	624	24.469	51.937	0.998	1.00	17.21	BTKA
ATOM	1833	CG	GLU	624	22.974	51.725	0.755	1.00	19.41	BTKA
ATOM	1834	CD	GLU	624	22.452	52.478	-0.459	1.00	18.43	BTKA
ATOM	1835	OE1	GLU	624	21.396	53.129	-0.339	1.00	16.44	BTKA
ATOM	1836	OE2	GLU	624	23.083	52.406	-1.539	1.00	21.39	BTKA
ATOM	1837	C	GLU	624	24.937	49.499	1.241	1.00	16.27	BTKA
ATOM	1838	O	GLU	624	23.935	48.824	1.451	1.00	20.19	BTKA
ATOM	1839	N	LYS	625	25.933	49.111	0.447	1.00	15.04	BTKA
ATOM	1840	CA	LYS	625	25.955	47.832	-0.251	1.00	14.80	BTKA
ATOM	1841	CB	LYS	625	26.989	47.874	-1.379	1.00	15.10	BTKA
ATOM	1842	CG	LYS	625	26.462	48.451	-2.693	1.00	19.31	BTKA
ATOM	1843	CD	LYS	625	25.903	49.878	-2.565	1.00	22.31	BTKA
ATOM	1844	CE	LYS	625	26.977	50.965	-2.680	1.00	21.63	BTKA
ATOM	1845	NZ	LYS	625	27.815	51.133	-1.465	1.00	17.99	BTKA
ATOM	1846	C	LYS	625	26.253	46.667	0.702	1.00	15.85	BTKA
ATOM	1847	O	LYS	625	25.563	45.645	0.678	1.00	16.83	BTKA
ATOM	1848	N	VAL	626	27.275	46.828	1.539	1.00	13.15	BTKA
ATOM	1849	CA	VAL	626	27.648	45.803	2.502	1.00	8.16	BTKA
ATOM	1850	CB	VAL	626	28.954	46.166	3.228	1.00	4.19	BTKA

	Atom Number	Atom Type	Amino Acid Residue		X	Y	Z	Occ.	Temp Factor	
ATOM	1851	CG1	VAL	626	29.170	45.266	4.437	1.00	9.56	BTKA
ATOM	1852	CG2	VAL	626	30.127	46.037	2.264	1.00	2.00	BTKA
ATOM	1853	C	VAL	626	26.523	45.649	3.508	1.00	10.56	BTKA
ATOM	1854	O	VAL	626	26.211	44.538	3.947	1.00	15.38	BTKA
ATOM	1855	N	TYR	627	25.870	46.754	3.837	1.00	11.00	BTKA
ATOM	1856	CA	TYR	627	24.774	46.696	4.791	1.00	6.70	BTKA
ATOM	1857	CB	TYR	627	24.406	48.089	5.303	1.00	5.85	BTKA
ATOM	1858	CG	TYR	627	23.438	48.052	6.462	1.00	5.63	BTKA
ATOM	1859	CD1	TYR	627	23.826	47.547	7.699	1.00	5.65	BTKA
ATOM	1860	CE1	TYR	627	22.943	47.500	8.765	1.00	3.44	BTKA
ATOM	1861	CD2	TYR	627	22.133	48.510	6.320	1.00	5.85	BTKA
ATOM	1862	CE2	TYR	627	21.237	48.465	7.383	1.00	7.61	BTKA
ATOM	1863	CZ	TYR	627	21.649	47.960	8.601	1.00	4.93	BTKA
ATOM	1864	OH	TYR	627	20.768	47.925	9.657	1.00	9.76	BTKA
ATOM	1865	C	TYR	627	23.566	46.005	4.182	1.00	2.00	BTKA
ATOM	1866	O	TYR	627	22.816	45.355	4.884	1.00	7.93	BTKA
ATOM	1867	N	THR	628	23.407	46.106	2.871	1.00	4.56	BTKA
ATOM	1868	CA	THR	628	22.293	45.463	2.189	1.00	6.68	BTKA
ATOM	1869	CB	THR	628	22.226	45.882	0.704	1.00	12.25	BTKA
ATOM	1870	OG1	THR	628	21.878	47.270	0.608	1.00	11.09	BTKA
ATOM	1871	CG2	THR	628	21.196	45.057	-0.043	1.00	12.83	BTKA
ATOM	1872	C	THR	628	22.382	43.938	2.284	1.00	3.84	BTKA
ATOM	1873	O	THR	628	21.372	43.266	2.450	1.00	2.00	BTKA
ATOM	1874	N	ILE	629	23.586	43.389	2.197	1.00	6.46	BTKA
ATOM	1875	CA	ILE	629	23.728	41.941	2.274	1.00	7.81	BTKA
ATOM	1876	CB	ILE	629	25.067	41.425	1.645	1.00	8.16	BTKA
ATOM	1877	CG2	ILE	629	25.040	41.634	0.154	1.00	5.31	BTKA
ATOM	1878	CG1	ILE	629	26.287	42.154	2.207	1.00	12.39	BTKA
ATOM	1879	CD	ILE	629	27.561	41.905	1.398	1.00	16.00	BTKA
ATOM	1880	C	ILE	629	23.482	41.373	3.676	1.00	7.41	BTKA
ATOM	1881	O	ILE	629	22.753	40.385	3.829	1.00	5.64	BTKA
ATOM	1882	N	MET	630	24.014	42.025	4.705	1.00	6.37	BTKA
ATOM	1883	CA	MET	630	23.790	41.527	6.052	1.00	8.30	BTKA
ATOM	1884	CB	MET	630	24.765	42.147	7.057	1.00	9.46	BTKA
ATOM	1885	CG	MET	630	24.540	43.605	7.371	1.00	12.86	BTKA
ATOM	1886	SD	MET	630	25.803	44.178	8.496	1.00	14.55	BTKA
ATOM	1887	CE	MET	630	24.866	44.657	9.833	1.00	15.03	BTKA
ATOM	1888	C	MET	630	22.344	41.777	6.472	1.00	9.78	BTKA
ATOM	1889	O	MET	630	21.709	40.917	7.084	1.00	13.22	BTKA
ATOM	1890	N	TYR	631	21.794	42.920	6.080	1.00	9.86	BTKA
ATOM	1891	CA	TYR	631	20.420	43.235	6.446	1.00	9.86	BTKA
ATOM	1892	CB	TYR	631	20.040	44.662	6.028	1.00	10.36	BTKA
ATOM	1893	CG	TYR	631	18.706	45.099	6.592	1.00	16.09	BTKA
ATOM	1894	CD1	TYR	631	17.519	44.790	5.929	1.00	17.24	BTKA
ATOM	1895	CE1	TYR	631	16.283	45.124	6.463	1.00	15.16	BTKA
ATOM	1896	CD2	TYR	631	18.622	45.768	7.811	1.00	14.11	BTKA
ATOM	1897	CE2	TYR	631	17.380	46.112	8.359	1.00	17.22	BTKA
ATOM	1898	CZ	TYR	631	16.218	45.784	7.674	1.00	16.41	BTKA
ATOM	1899	OH	TYR	631	14.975	46.120	8.166	1.00	18.16	BTKA
ATOM	1900	C	TYR	631	19.415	42.228	5.892	1.00	10.69	BTKA
ATOM	1901	O	TYR	631	18.403	41.949	6.532	1.00	12.38	BTKA
ATOM	1902	N	SER	632	19.698	41.666	4.721	1.00	9.17	BTKA
ATOM	1903	CA	SER	632	18.796	40.692	4.113	1.00	10.83	BTKA
ATOM	1904	CB	SER	632	19.314	40.280	2.728	1.00	6.49	BTKA
ATOM	1905	OG	SER	632	20.564	39.615	2.807	1.00	2.00	BTKA
ATOM	1906	C	SER	632	18.626	39.450	4.983	1.00	9.86	BTKA
ATOM	1907	O	SER	632	17.565	38.827	4.991	1.00	10.42	BTKA
ATOM	1908	N	CYS	633	19.667	39.117	5.740	1.00	11.03	BTKA

	Atom Number	Atom Type	Amino Acid Residue		X	Y	Z	Occ.	Temp Factor	
ATOM	1909	CA	CYS	633	19.677	37.933	6.599	1.00	7.43	BTKA
ATOM	1910	CB	CYS	633	21.060	37.759	7.231	1.00	6.63	BTKA
ATOM	1911	SG	CYS	633	22.373	37.428	6.045	1.00	4.09	BTKA
ATOM	1912	C	CYS	633	18.632	37.940	7.699	1.00	6.70	BTKA
ATOM	1913	O	CYS	633	18.215	36.888	8.177	1.00	8.11	BTKA
ATOM	1914	N	TRP	634	18.156	39.125	8.043	1.00	6.33	BTKA
ATOM	1915	CA	TRP	634	17.206	39.273	9.129	1.00	9.48	BTKA
ATOM	1916	CB	TRP	634	17.666	40.428	10.010	1.00	9.15	BTKA
ATOM	1917	CG	TRP	634	19.135	40.440	10.331	1.00	4.86	BTKA
ATOM	1918	CD2	TRP	634	19.974	41.590	10.376	1.00	3.49	BTKA
ATOM	1919	CE2	TRP	634	21.261	41.154	10.756	1.00	2.25	BTKA
ATOM	1920	CE3	TRP	634	19.770	42.955	10.140	1.00	3.18	BTKA
ATOM	1921	CD1	TRP	634	19.918	39.378	10.671	1.00	2.00	BTKA
ATOM	1922	NE1	TRP	634	21.197	39.797	10.930	1.00	2.34	BTKA
ATOM	1923	CZ2	TRP	634	22.332	42.035	10.904	1.00	2.00	BTKA
ATOM	1924	CZ3	TRP	634	20.835	43.827	10.291	1.00	2.00	BTKA
ATOM	1925	CH2	TRP	634	22.098	43.361	10.668	1.00	2.00	BTKA
ATOM	1926	C	TRP	634	15.768	39.537	8.697	1.00	10.94	BTKA
ATOM	1927	O	TRP	634	15.015	40.182	9.422	1.00	13.81	BTKA
ATOM	1928	N	HIS	635	15.340	38.956	7.588	1.00	11.56	BTKA
ATOM	1929	CA	HIS	635	13.997	39.231	7.090	1.00	13.40	BTKA
ATOM	1930	CB	HIS	635	13.833	38.692	5.670	1.00	8.93	BTKA
ATOM	1931	CG	HIS	635	12.712	39.336	4.923	1.00	7.82	BTKA
ATOM	1932	CD2	HIS	635	12.720	40.264	3.936	1.00	9.65	BTKA
ATOM	1933	ND1	HIS	635	11.386	39.124	5.236	1.00	6.04	BTKA
ATOM	1934	CE1	HIS	635	10.627	39.896	4.484	1.00	6.47	BTKA
ATOM	1935	NE2	HIS	635	11.410	40.598	3.687	1.00	11.66	BTKA
ATOM	1936	C	HIS	635	12.720	38.940	7.888	1.00	16.55	BTKA
ATOM	1937	O	HIS	635	11.689	39.543	7.589	1.00	21.21	BTKA
ATOM	1938	N	GLU	636	12.758	38.053	8.877	1.00	16.72	BTKA
ATOM	1939	CA	GLU	636	11.563	37.677	9.675	1.00	16.32	BTKA
ATOM	1940	CB	GLU	636	10.524	38.810	9.812	1.00	18.59	BTKA
ATOM	1941	CG	GLU	636	9.347	38.458	10.730	1.00	25.85	BTKA
ATOM	1942	CD	GLU	636	8.003	39.015	10.258	1.00	28.55	BTKA
ATOM	1943	OE1	GLU	636	7.772	39.080	9.030	1.00	29.75	BTKA
ATOM	1944	OE2	GLU	636	7.161	39.364	11.115	1.00	28.67	BTKA
ATOM	1945	C	GLU	636	10.925	36.492	8.966	1.00	16.71	BTKA
ATOM	1946	O	GLU	636	10.924	35.384	9.492	1.00	19.32	BTKA
ATOM	1947	N	LYS	637	10.385	36.728	7.773	1.00	16.09	BTKA
ATOM	1948	CA	LYS	637	9.798	35.654	6.979	1.00	15.70	BTKA
ATOM	1949	CB	LYS	637	9.072	36.210	5.740	1.00	14.04	BTKA
ATOM	1950	CG	LYS	637	8.061	37.320	6.012	1.00	14.27	BTKA
ATOM	1951	CD	LYS	637	6.625	36.817	6.109	1.00	21.34	BTKA
ATOM	1952	CE	LYS	637	6.472	35.700	7.120	1.00	21.37	BTKA
ATOM	1953	NZ	LYS	637	6.679	34.358	6.495	1.00	22.42	BTKA
ATOM	1954	C	LYS	637	10.996	34.830	6.510	1.00	15.02	BTKA
ATOM	1955	O	LYS	637	11.751	35.270	5.636	1.00	14.64	BTKA
ATOM	1956	N	ALA	638	11.190	33.665	7.116	1.00	12.71	BTKA
ATOM	1957	CA	ALA	638	12.294	32.778	6.769	1.00	9.49	BTKA
ATOM	1958	CB	ALA	638	12.074	31.417	7.398	1.00	11.57	BTKA
ATOM	1959	C	ALA	638	12.574	32.621	5.270	1.00	12.33	BTKA
ATOM	1960	O	ALA	638	13.724	32.764	4.840	1.00	9.51	BTKA
ATOM	1961	N	ASP	639	11.526	32.378	4.475	1.00	11.12	BTKA
ATOM	1962	CA	ASP	639	11.678	32.163	3.030	1.00	11.04	BTKA
ATOM	1963	CB	ASP	639	10.431	31.478	2.426	1.00	13.90	BTKA
ATOM	1964	CG	ASP	639	9.181	32.358	2.437	1.00	13.58	BTKA
ATOM	1965	OD1	ASP	639	9.270	33.586	2.626	1.00	15.17	BTKA
ATOM	1966	OD2	ASP	639	8.081	31.808	2.235	1.00	15.41	BTKA

	Atom Number	Atom Type	Amino Acid Residue		X	Y	Z	Occ.	Temp Factor	
ATOM	1967	C	ASP	639	12.074	33.366	2.185	1.00	10.51	BTKA
ATOM	1968	O	ASP	639	12.206	33.258	0.962	1.00	3.89	BTKA
ATOM	1969	N	GLU	640	12.203	34.517	2.836	1.00	10.52	BTKA
ATOM	1970	CA	GLU	640	12.575	35.754	2.169	1.00	11.19	BTKA
ATOM	1971	CB	GLU	640	11.673	36.892	2.640	1.00	14.28	BTKA
ATOM	1972	CG	GLU	640	11.180	37.808	1.531	1.00	24.80	BTKA
ATOM	1973	CD	GLU	640	9.741	37.523	1.125	1.00	30.36	BTKA
ATOM	1974	OE1	GLU	640	9.499	37.238	-0.072	1.00	34.01	BTKA
ATOM	1975	OE2	GLU	640	8.849	37.602	2.002	1.00	36.33	BTKA
ATOM	1976	C	GLU	640	14.030	36.074	2.496	1.00	9.22	BTKA
ATOM	1977	O	GLU	640	14.556	37.117	2.120	1.00	10.28	BTKA
ATOM	1978	N	ARG	641	14.658	35.185	3.249	1.00	8.49	BTKA
ATOM	1979	CA	ARG	641	16.048	35.343	3.626	1.00	10.21	BTKA
ATOM	1980	CB	ARG	641	16.256	34.861	5.069	1.00	8.41	BTKA
ATOM	1981	CG	ARG	641	15.151	35.391	5.991	1.00	10.60	BTKA
ATOM	1982	CD	ARG	641	15.623	35.692	7.392	1.00	13.17	BTKA
ATOM	1983	NE	ARG	641	15.831	34.497	8.189	1.00	18.11	BTKA
ATOM	1984	CZ	ARG	641	14.942	34.007	9.045	1.00	15.39	BTKA
ATOM	1985	NH1	ARG	641	13.776	34.608	9.222	1.00	14.59	BTKA
ATOM	1986	NH2	ARG	641	15.228	32.917	9.734	1.00	13.36	BTKA
ATOM	1987	C	ARG	641	16.834	34.519	2.608	1.00	11.06	BTKA
ATOM	1988	O	ARG	641	16.490	33.367	2.320	1.00	8.77	BTKA
ATOM	1989	N	PRO	642	17.843	35.141	1.982	1.00	11.46	BTKA
ATOM	1990	CD	PRO	642	18.197	36.544	2.242	1.00	10.26	BTKA
ATOM	1991	CA	PRO	642	18.733	34.573	0.961	1.00	13.85	BTKA
ATOM	1992	CB	PRO	642	19.725	35.710	0.721	1.00	16.79	BTKA
ATOM	1993	CG	PRO	642	18.897	36.914	0.967	1.00	15.67	BTKA
ATOM	1994	C	PRO	642	19.471	33.301	1.348	1.00	12.77	BTKA
ATOM	1995	O	PRO	642	19.570	32.959	2.522	1.00	11.54	BTKA
ATOM	1996	N	THR	643	19.977	32.597	0.342	1.00	11.30	BTKA
ATOM	1997	CA	THR	643	20.747	31.389	0.580	1.00	10.65	BTKA
ATOM	1998	CB	THR	643	20.667	30.414	-0.614	1.00	6.97	BTKA
ATOM	1999	OG1	THR	643	21.115	31.067	-1.807	1.00	10.04	BTKA
ATOM	2000	CG2	THR	643	19.255	29.934	-0.813	1.00	8.33	BTKA
ATOM	2001	C	THR	643	22.201	31.829	0.778	1.00	10.25	BTKA
ATOM	2002	O	THR	643	22.545	32.983	0.520	1.00	13.36	BTKA
ATOM	2003	N	PHE	644	23.044	30.920	1.255	1.00	9.85	BTKA
ATOM	2004	CA	PHE	644	24.454	31.223	1.459	1.00	8.80	BTKA
ATOM	2005	CB	PHE	644	25.125	30.152	2.314	1.00	6.23	BTKA
ATOM	2006	CG	PHE	644	24.910	30.343	3.782	1.00	7.15	BTKA
ATOM	2007	CD1	PHE	644	25.331	31.515	4.405	1.00	9.73	BTKA
ATOM	2008	CD2	PHE	644	24.268	29.367	4.543	1.00	4.29	BTKA
ATOM	2009	CE1	PHE	644	25.117	31.715	5.766	1.00	9.97	BTKA
ATOM	2010	CE2	PHE	644	24.048	29.554	5.900	1.00	2.00	BTKA
ATOM	2011	CZ	PHE	644	24.473	30.732	6.515	1.00	8.09	BTKA
ATOM	2012	C	PHE	644	25.175	31.387	0.136	1.00	6.83	BTKA
ATOM	2013	O	PHE	644	26.132	32.146	0.042	1.00	6.14	BTKA
ATOM	2014	N	ALA	645	24.679	30.703	-0.893	1.00	10.54	BTKA
ATOM	2015	CA	ALA	645	25.247	30.791	-2.241	1.00	9.84	BTKA
ATOM	2016	CB	ALA	645	24.635	29.730	-3.150	1.00	14.63	BTKA
ATOM	2017	C	ALA	645	24.976	32.179	-2.809	1.00	9.74	BTKA
ATOM	2018	O	ALA	645	25.815	32.751	-3.512	1.00	11.66	BTKA
ATOM	2019	N	ILE	646	23.787	32.705	-2.534	1.00	10.19	BTKA
ATOM	2020	CA	ILE	646	23.434	34.029	-3.015	1.00	9.44	BTKA
ATOM	2021	CB	ILE	646	21.912	34.306	-2.904	1.00	10.35	BTKA
ATOM	2022	CG2	ILE	646	21.615	35.788	-3.117	1.00	9.73	BTKA
ATOM	2023	CG1	ILE	646	21.163	33.467	-3.945	1.00	12.53	BTKA
ATOM	2024	CD	ILE	646	19.749	33.935	-4.220	1.00	10.68	BTKA

	Atom Number	Atom Type	Amino Acid Residue		X	Y	Z	Occ.	Temp Factor	
ATOM	2025	C	ILE	646	24.237	35.057	-2.234	1.00	8.64	BTKA
ATOM	2026	O	ILE	646	24.792	35.987	-2.820	1.00	12.42	BTKA
ATOM	2027	N	LEU	647	24.329	34.870	-0.923	1.00	5.16	BTKA
ATOM	2028	CA	LEU	647	25.096	35.777	-0.076	1.00	5.21	BTKA
ATOM	2029	CB	LEU	647	25.049	35.331	1.383	1.00	6.62	BTKA
ATOM	2030	CG	LEU	647	23.782	35.668	2.152	1.00	2.00	BTKA
ATOM	2031	CD1	LEU	647	23.785	34.910	3.454	1.00	7.11	BTKA
ATOM	2032	CD2	LEU	647	23.705	37.180	2.390	1.00	6.32	BTKA
ATOM	2033	C	LEU	647	26.538	35.803	-0.538	1.00	4.59	BTKA
ATOM	2034	O	LEU	647	27.151	36.859	-0.615	1.00	9.34	BTKA
ATOM	2035	N	LEU	648	27.083	34.632	-0.838	1.00	6.10	BTKA
ATOM	2036	CA	LEU	648	28.454	34.540	-1.307	1.00	7.56	BTKA
ATOM	2037	CB	LEU	648	28.901	33.087	-1.407	1.00	6.76	BTKA
ATOM	2038	CG	LEU	648	30.313	32.904	-1.953	1.00	5.57	BTKA
ATOM	2039	CD1	LEU	648	31.338	33.392	-0.951	1.00	8.87	BTKA
ATOM	2040	CD2	LEU	648	30.531	31.456	-2.262	1.00	9.05	BTKA
ATOM	2041	C	LEU	648	28.603	35.218	-2.662	1.00	7.15	BTKA
ATOM	2042	O	LEU	648	29.619	35.860	-2.914	1.00	5.11	BTKA
ATOM	2043	N	SER	649	27.606	35.079	-3.535	1.00	7.37	BTKA
ATOM	2044	CA	SER	649	27.684	35.715	-4.848	1.00	11.39	BTKA
ATOM	2045	CB	SER	649	26.619	35.172	-5.826	1.00	13.66	BTKA
ATOM	2046	OG	SER	649	25.352	35.803	-5.718	1.00	18.95	BTKA
ATOM	2047	C	SER	649	27.588	37.226	-4.674	1.00	13.90	BTKA
ATOM	2048	O	SER	649	28.255	37.979	-5.384	1.00	14.33	BTKA
ATOM	2049	N	ASN	650	26.813	37.666	-3.685	1.00	15.59	BTKA
ATOM	2050	CA	ASN	650	26.669	39.097	-3.418	1.00	14.80	BTKA
ATOM	2051	CB	ASN	650	25.655	39.351	-2.301	1.00	15.49	BTKA
ATOM	2052	CG	ASN	650	24.218	39.195	-2.758	1.00	13.88	BTKA
ATOM	2053	OD1	ASN	650	23.911	39.333	-3.941	1.00	16.71	BTKA
ATOM	2054	ND2	ASN	650	23.323	38.920	-1.814	1.00	18.03	BTKA
ATOM	2055	C	ASN	650	28.035	39.590	-2.975	1.00	16.71	BTKA
ATOM	2056	O	ASN	650	28.627	40.461	-3.602	1.00	18.95	BTKA
ATOM	2057	N	ILE	651	28.553	38.972	-1.920	1.00	17.37	BTKA
ATOM	2058	CA	ILE	651	29.856	39.315	-1.368	1.00	16.71	BTKA
ATOM	2059	CB	ILE	651	30.300	38.269	-0.330	1.00	16.01	BTKA
ATOM	2060	CG2	ILE	651	31.766	38.473	0.049	1.00	16.81	BTKA
ATOM	2061	CG1	ILE	651	29.397	38.333	0.902	1.00	18.86	BTKA
ATOM	2062	CD	ILE	651	29.787	37.353	1.998	1.00	18.13	BTKA
ATOM	2063	C	ILE	651	30.936	39.407	-2.441	1.00	17.88	BTKA
ATOM	2064	O	ILE	651	31.730	40.340	-2.442	1.00	17.27	BTKA
ATOM	2065	N	LEU	652	30.979	38.425	-3.333	1.00	17.38	BTKA
ATOM	2066	CA	LEU	652	31.988	38.410	-4.383	1.00	16.93	BTKA
ATOM	2067	CB	LEU	652	31.927	37.097	-5.174	1.00	16.89	BTKA
ATOM	2068	CG	LEU	652	32.426	35.821	-4.496	1.00	14.36	BTKA
ATOM	2069	CD1	LEU	652	32.223	34.644	-5.415	1.00	17.00	BTKA
ATOM	2070	CD2	LEU	652	33.890	35.966	-4.155	1.00	17.94	BTKA
ATOM	2071	C	LEU	652	31.864	39.593	-5.339	1.00	17.77	BTKA
ATOM	2072	O	LEU	652	32.869	40.153	-5.775	1.00	14.19	BTKA
ATOM	2073	N	ASP	653	30.626	39.958	-5.660	1.00	16.94	BTKA
ATOM	2074	CA	ASP	653	30.338	41.052	-6.583	1.00	18.91	BTKA
ATOM	2075	CB	ASP	653	28.839	41.029	-6.933	1.00	22.19	BTKA
ATOM	2076	CG	ASP	653	28.511	41.768	-8.220	1.00	27.15	BTKA
ATOM	2077	OD1	ASP	653	28.383	43.014	-8.190	1.00	26.08	BTKA
ATOM	2078	OD2	ASP	653	28.338	41.094	-9.261	1.00	29.58	BTKA
ATOM	2079	C	ASP	653	30.743	42.397	-5.971	1.00	16.94	BTKA
ATOM	2080	O	ASP	653	30.021	42.968	-5.153	1.00	18.07	BTKA
ATOM	2081	N	VAL	654	31.910	42.883	-6.363	1.00	17.09	BTKA
ATOM	2082	CA	VAL	654	32.448	44.156	-5.873	1.00	19.99	BTKA

	Atom Number	Atom Type	Amino Acid Residue		X	Y	Z	Occ.	Temp Factor	
ATOM	2083	CB	VAL	654	32.525	44.192	-4.285	1.00	15.42	BTKA
ATOM	2084	CG1	VAL	654	33.538	43.189	-3.741	1.00	19.20	BTKA
ATOM	2085	CG2	VAL	654	32.836	45.587	-3.792	1.00	15.46	BTKA
ATOM	2086	C	VAL	654	33.831	44.409	-6.521	1.00	21.38	BTKA
ATOM	2087	OT1	VAL	654	34.043	45.515	-7.073	1.00	20.29	BTKA
ATOM	2088	OT2	VAL	654	34.668	43.475	-6.533	1.00	23.32	BTKA
TER	2088		VAL	654						BTKA
ATOM	2089	CB	ILE	397	34.822	44.259	42.166	1.00	28.06	BTKB
ATOM	2090	CG2	ILE	397	35.367	43.761	43.501	1.00	30.24	BTKB
ATOM	2091	CG1	ILE	397	33.354	44.660	42.302	1.00	27.51	BTKB
ATOM	2092	CD	ILE	397	32.460	43.563	42.838	1.00	31.05	BTKB
ATOM	2093	C	ILE	397	37.125	45.091	41.610	1.00	29.53	BTKB
ATOM	2094	O	ILE	397	37.977	45.873	42.022	1.00	31.32	BTKB
ATOM	2095	N	ILE	397	35.200	45.884	40.296	1.00	27.80	BTKB
ATOM	2096	CA	ILE	397	35.647	45.461	41.653	1.00	29.30	BTKB
ATOM	2097	N	ASP	398	37.413	43.917	41.052	1.00	29.94	BTKB
ATOM	2098	CA	ASP	398	38.771	43.396	40.924	1.00	28.21	BTKB
ATOM	2099	CB	ASP	398	38.711	41.951	40.409	1.00	27.14	BTKB
ATOM	2100	CG	ASP	398	40.055	41.431	39.939	1.00	28.88	BTKB
ATOM	2101	OD1	ASP	398	40.805	40.866	40.760	1.00	29.93	BTKB
ATOM	2102	OD2	ASP	398	40.353	41.565	38.735	1.00	29.99	BTKB
ATOM	2103	C	ASP	398	39.631	44.248	39.999	1.00	30.83	BTKB
ATOM	2104	O	ASP	398	39.299	44.428	38.823	1.00	28.34	BTKB
ATOM	2105	N	PRO	399	40.726	44.819	40.529	1.00	30.97	BTKB
ATOM	2106	CD	PRO	399	41.104	44.844	41.953	1.00	29.33	BTKB
ATOM	2107	CA	PRO	399	41.633	45.654	39.735	1.00	30.72	BTKB
ATOM	2108	CB	PRO	399	42.689	46.073	40.760	1.00	33.06	BTKB
ATOM	2109	CG	PRO	399	41.908	46.118	42.044	1.00	32.66	BTKB
ATOM	2110	C	PRO	399	42.236	44.809	38.611	1.00	30.41	BTKB
ATOM	2111	O	PRO	399	43.229	44.106	38.808	1.00	27.77	BTKB
ATOM	2112	N	LYS	400	41.618	44.906	37.435	1.00	31.71	BTKB
ATOM	2113	CA	LYS	400	41.991	44.169	36.225	1.00	32.73	BTKB
ATOM	2114	CB	LYS	400	41.466	44.913	34.992	1.00	31.73	BTKB
ATOM	2115	CG	LYS	400	41.243	44.014	33.789	1.00	31.68	BTKB
ATOM	2116	CD	LYS	400	40.893	44.804	32.545	1.00	29.01	BTKB
ATOM	2117	CE	LYS	400	40.459	43.882	31.409	1.00	27.04	BTKB
ATOM	2118	NZ	LYS	400	39.176	43.195	31.722	1.00	25.44	BTKB
ATOM	2119	C	LYS	400	43.453	43.746	35.993	1.00	35.08	BTKB
ATOM	2120	O	LYS	400	43.710	42.872	35.157	1.00	32.76	BTKB
ATOM	2121	N	ASP	401	44.410	44.363	36.684	1.00	37.73	BTKB
ATOM	2122	CA	ASP	401	45.807	43.987	36.493	1.00	38.72	BTKB
ATOM	2123	CB	ASP	401	46.682	45.209	36.209	1.00	38.08	BTKB
ATOM	2124	CG	ASP	401	48.080	44.824	35.748	1.00	38.22	BTKB
ATOM	2125	OD1	ASP	401	48.992	44.757	36.599	1.00	39.11	BTKB
ATOM	2126	OD2	ASP	401	48.262	44.564	34.539	1.00	40.47	BTKB
ATOM	2127	C	ASP	401	46.375	43.195	37.668	1.00	40.61	BTKB
ATOM	2128	O	ASP	401	46.429	43.683	38.802	1.00	39.92	BTKB
ATOM	2129	N	LEU	402	46.832	41.982	37.365	1.00	39.68	BTKB
ATOM	2130	CA	LEU	402	47.412	41.076	38.347	1.00	35.79	BTKB
ATOM	2131	CB	LEU	402	46.300	40.318	39.083	1.00	30.36	BTKB
ATOM	2132	CG	LEU	402	45.296	39.475	38.286	1.00	25.43	BTKB
ATOM	2133	CD1	LEU	402	44.710	38.416	39.200	1.00	25.89	BTKB
ATOM	2134	CD2	LEU	402	44.189	40.326	37.678	1.00	19.90	BTKB
ATOM	2135	C	LEU	402	48.339	40.090	37.627	1.00	36.68	BTKB
ATOM	2136	O	LEU	402	48.350	40.034	36.396	1.00	37.32	BTKB
ATOM	2137	N	THR	403	49.128	39.332	38.385	1.00	38.28	BTKB
ATOM	2138	CA	THR	403	50.047	38.356	37.798	1.00	39.00	BTKB
ATOM	2139	CB	THR	403	50.922	37.688	38.885	1.00	38.43	BTKB

Atom Number	Atom Type	Amino Acid Residue		X	Y	Z	Occ.	Temp Factor	
ATOM 2140	OG1	THR	403	51.318	38.666	39.857	1.00	39.19	BTKB
ATOM 2141	CG2	THR	403	52.165	37.073	38.262	1.00	34.76	BTKB
ATOM 2142	C	THR	403	49.258	37.270	37.050	1.00	41.52	BTKB
ATOM 2143	O	THR	403	48.103	36.993	37.392	1.00	43.01	BTKB
ATOM 2144	N	PHE	404	49.884	36.663	36.041	1.00	40.42	BTKB
ATOM 2145	CA	PHE	404	49.262	35.613	35.226	1.00	38.98	BTKB
ATOM 2146	CB	PHE	404	48.349	36.210	34.143	1.00	38.33	BTKB
ATOM 2147	CG	PHE	404	48.701	37.620	33.748	1.00	39.41	BTKB
ATOM 2148	CD1	PHE	404	47.704	38.578	33.617	1.00	39.35	BTKB
ATOM 2149	CD2	PHE	404	50.026	38.000	33.542	1.00	40.12	BTKB
ATOM 2150	CE1	PHE	404	48.016	39.892	33.293	1.00	39.05	BTKB
ATOM 2151	CE2	PHE	404	50.351	39.314	33.218	1.00	39.92	BTKB
ATOM 2152	CZ	PHE	404	49.344	40.261	33.094	1.00	41.14	BTKB
ATOM 2153	C	PHE	404	50.316	34.723	34.578	1.00	38.11	BTKB
ATOM 2154	O	PHE	404	51.263	35.217	33.974	1.00	38.10	BTKB
ATOM 2155	N	LEU	405	50.151	33.412	34.722	1.00	39.17	BTKB
ATOM 2156	CA	LEU	405	51.096	32.450	34.168	1.00	38.13	BTKB
ATOM 2157	CB	LEU	405	51.676	31.575	35.285	1.00	39.62	BTKB
ATOM 2158	CG	LEU	405	52.874	32.193	36.020	1.00	42.57	BTKB
ATOM 2159	CD1	LEU	405	53.105	31.533	37.378	1.00	41.80	BTKB
ATOM 2160	CD2	LEU	405	54.112	32.086	35.140	1.00	40.80	BTKB
ATOM 2161	C	LEU	405	50.504	31.596	33.050	1.00	36.37	BTKB
ATOM 2162	O	LEU	405	50.680	31.910	31.872	1.00	38.19	BTKB
ATOM 2163	N	LYS	406	49.832	30.506	33.398	1.00	33.49	BTKB
ATOM 2164	CA	LYS	406	49.229	29.657	32.379	1.00	31.11	BTKB
ATOM 2165	CB	LYS	406	49.715	28.201	32.487	1.00	32.83	BTKB
ATOM 2166	CG	LYS	406	49.155	27.413	33.671	1.00	31.89	BTKB
ATOM 2167	CD	LYS	406	49.709	25.994	33.712	1.00	29.73	BTKB
ATOM 2168	CE	LYS	406	49.132	25.197	34.874	1.00	25.18	BTKB
ATOM 2169	NZ	LYS	406	47.664	24.987	34.754	1.00	23.18	BTKB
ATOM 2170	C	LYS	406	47.721	29.727	32.544	1.00	31.03	BTKB
ATOM 2171	O	LYS	406	47.194	30.685	33.126	1.00	29.59	BTKB
ATOM 2172	N	GLU	407	47.038	28.689	32.075	1.00	28.47	BTKB
ATOM 2173	CA	GLU	407	45.592	28.615	32.145	1.00	24.70	BTKB
ATOM 2174	CB	GLU	407	45.028	28.721	30.723	1.00	25.09	BTKB
ATOM 2175	CG	GLU	407	43.575	29.148	30.632	1.00	27.67	BTKB
ATOM 2176	CD	GLU	407	42.666	28.087	30.062	1.00	28.92	BTKB
ATOM 2177	OE1	GLU	407	41.443	28.231	30.229	1.00	30.56	BTKB
ATOM 2178	OE2	GLU	407	43.157	27.114	29.450	1.00	32.96	BTKB
ATOM 2179	C	GLU	407	45.220	27.272	32.764	1.00	22.29	BTKB
ATOM 2180	O	GLU	407	46.096	26.485	33.116	1.00	24.55	BTKB
ATOM 2181	N	LEU	408	43.924	27.037	32.924	1.00	21.71	BTKB
ATOM 2182	CA	LEU	408	43.411	25.787	33.470	1.00	21.08	BTKB
ATOM 2183	CB	LEU	408	42.611	26.020	34.751	1.00	20.12	BTKB
ATOM 2184	CG	LEU	408	43.312	25.979	36.104	1.00	17.11	BTKB
ATOM 2185	CD1	LEU	408	44.189	27.196	36.305	1.00	16.68	BTKB
ATOM 2186	CD2	LEU	408	42.244	25.924	37.169	1.00	20.38	BTKB
ATOM 2187	C	LEU	408	42.513	25.113	32.444	1.00	21.69	BTKB
ATOM 2188	O	LEU	408	42.883	24.088	31.872	1.00	25.66	BTKB
ATOM 2189	N	GLY	409	41.345	25.697	32.191	1.00	26.47	BTKB
ATOM 2190	CA	GLY	409	40.426	25.099	31.233	1.00	30.31	BTKB
ATOM 2191	C	GLY	409	39.026	25.681	31.179	1.00	31.13	BTKB
ATOM 2192	O	GLY	409	38.864	26.839	30.800	1.00	28.40	BTKB
ATOM 2193	N	THR	410	38.023	24.897	31.586	1.00	34.19	BTKB
ATOM 2194	CA	THR	410	36.623	25.337	31.563	1.00	35.54	BTKB
ATOM 2195	CB	THR	410	35.974	25.015	30.188	1.00	39.00	BTKB
ATOM 2196	OG1	THR	410	36.807	25.525	29.140	1.00	42.12	BTKB
ATOM 2197	CG2	THR	410	34.576	25.635	30.069	1.00	36.90	BTKB

	Atom Number	Atom Type	Amino Acid Residue		X	Y	Z	Occ.	Temp Factor	
ATOM	2198	C	THR	410	35.758	24.713	32.673	1.00	34.43	BTKB
ATOM	2199	O	THR	410	36.028	23.601	33.141	1.00	31.80	BTKB
ATOM	2200	N	GLY	411	34.721	25.447	33.076	1.00	33.66	BTKB
ATOM	2201	CA	GLY	411	33.801	24.986	34.102	1.00	32.04	BTKB
ATOM	2202	C	GLY	411	32.351	25.093	33.645	1.00	32.34	BTKB
ATOM	2203	O	GLY	411	31.738	24.093	33.280	1.00	33.64	BTKB
ATOM	2204	N	GLN	412	31.811	26.308	33.623	1.00	31.61	BTKB
ATOM	2205	CA	GLN	412	30.426	26.513	33.207	1.00	28.88	BTKB
ATOM	2206	CB	GLN	412	29.567	26.874	34.418	1.00	30.03	BTKB
ATOM	2207	CG	GLN	412	28.212	26.192	34.445	1.00	31.90	BTKB
ATOM	2208	CD	GLN	412	28.294	24.745	34.891	1.00	31.28	BTKB
ATOM	2209	OE1	GLN	412	29.317	24.084	34.715	1.00	31.63	BTKB
ATOM	2210	NE2	GLN	412	27.217	24.250	35.493	1.00	28.67	BTKB
ATOM	2211	C	GLN	412	30.270	27.600	32.140	1.00	28.86	BTKB
ATOM	2212	O	GLN	412	29.267	27.638	31.418	1.00	28.11	BTKB
ATOM	2213	N	PHE	413	31.234	28.512	32.074	1.00	28.97	BTKB
ATOM	2214	CA	PHE	413	31.188	29.593	31.097	1.00	28.08	BTKB
ATOM	2215	CB	PHE	413	31.388	30.954	31.773	1.00	28.79	BTKB
ATOM	2216	CG	PHE	413	30.221	31.403	32.594	1.00	26.11	BTKB
ATOM	2217	CD1	PHE	413	29.317	32.325	32.084	1.00	30.79	BTKB
ATOM	2218	CD2	PHE	413	30.023	30.904	33.872	1.00	29.49	BTKB
ATOM	2219	CE1	PHE	413	28.229	32.740	32.833	1.00	33.14	BTKB
ATOM	2220	CE2	PHE	413	28.935	31.313	34.633	1.00	31.02	BTKB
ATOM	2221	CZ	PHE	413	28.036	32.234	34.113	1.00	33.86	BTKB
ATOM	2222	C	PHE	413	32.248	29.403	30.027	1.00	30.53	BTKB
ATOM	2223	O	PHE	413	31.989	28.797	28.987	1.00	34.18	BTKB
ATOM	2224	N	GLY	414	33.453	29.889	30.306	1.00	29.58	BTKB
ATOM	2225	CA	GLY	414	34.527	29.781	29.343	1.00	29.36	BTKB
ATOM	2226	C	GLY	414	35.824	29.289	29.938	1.00	30.73	BTKB
ATOM	2227	O	GLY	414	35.824	28.404	30.806	1.00	29.03	BTKB
ATOM	2228	N	VAL	415	36.918	29.917	29.507	1.00	31.12	BTKB
ATOM	2229	CA	VAL	415	38.273	29.569	29.930	1.00	29.86	BTKB
ATOM	2230	CB	VAL	415	39.292	29.895	28.818	1.00	28.63	BTKB
ATOM	2231	CG1	VAL	415	39.093	28.976	27.636	1.00	20.44	BTKB
ATOM	2232	CG2	VAL	415	39.158	31.341	28.388	1.00	28.08	BTKB
ATOM	2233	C	VAL	415	38.773	30.174	31.247	1.00	33.07	BTKB
ATOM	2234	O	VAL	415	38.753	31.395	31.441	1.00	34.75	BTKB
ATOM	2235	N	VAL	416	39.268	29.307	32.125	1.00	33.11	BTKB
ATOM	2236	CA	VAL	416	39.792	29.716	33.426	1.00	33.57	BTKB
ATOM	2237	CB	VAL	416	39.158	28.867	34.561	1.00	36.44	BTKB
ATOM	2238	CG1	VAL	416	39.077	27.402	34.147	1.00	38.53	BTKB
ATOM	2239	CG2	VAL	416	39.944	29.014	35.860	1.00	36.43	BTKB
ATOM	2240	C	VAL	416	41.326	29.621	33.437	1.00	32.35	BTKB
ATOM	2241	O	VAL	416	41.880	28.539	33.264	1.00	32.92	BTKB
ATOM	2242	N	LYS	417	42.000	30.762	33.595	1.00	28.13	BTKB
ATOM	2243	CA	LYS	417	43.470	30.834	33.601	1.00	22.76	BTKB
ATOM	2244	CB	LYS	417	43.920	32.071	32.810	1.00	21.32	BTKB
ATOM	2245	CG	LYS	417	43.060	32.342	31.574	1.00	24.74	BTKB
ATOM	2246	CD	LYS	417	43.513	33.567	30.806	1.00	23.99	BTKB
ATOM	2247	CE	LYS	417	42.534	33.946	29.710	1.00	15.58	BTKB
ATOM	2248	NZ	LYS	417	42.968	35.229	29.104	1.00	20.25	BTKB
ATOM	2249	C	LYS	417	44.014	30.895	35.031	1.00	18.43	BTKB
ATOM	2250	O	LYS	417	43.265	30.665	35.976	1.00	17.13	BTKB
ATOM	2251	N	ALA	418	45.298	31.214	35.195	1.00	14.44	BTKB
ATOM	2252	CA	ALA	418	45.898	31.301	36.533	1.00	18.16	BTKB
ATOM	2253	CB	ALA	418	46.737	30.057	36.834	1.00	18.21	BTKB
ATOM	2254	C	ALA	418	46.750	32.548	36.706	1.00	18.40	BTKB
ATOM	2255	O	ALA	418	47.448	32.962	35.783	1.00	19.90	BTKB

	Atom Number	Atom Type	Amino Acid Residue		X	Y	Z	Occ.	Temp Factor	
ATOM	2256	N	GLY	419	46.724	33.116	37.905	1.00	20.29	BTKB
ATOM	2257	CA	GLY	419	47.507	34.308	38.176	1.00	20.56	BTKB
ATOM	2258	C	GLY	419	47.617	34.626	39.651	1.00	22.74	BTKB
ATOM	2259	O	GLY	419	47.091	33.895	40.487	1.00	24.36	BTKB
ATOM	2260	N	ALA	420	48.305	35.712	39.982	1.00	23.32	BTKB
ATOM	2261	CA	ALA	420	48.460	36.110	41.378	1.00	23.35	BTKB
ATOM	2262	CB	ALA	420	49.927	36.125	41.774	1.00	23.90	BTKB
ATOM	2263	C	ALA	420	47.837	37.484	41.587	1.00	21.75	BTKB
ATOM	2264	O	ALA	420	48.198	38.448	40.912	1.00	24.80	BTKB
ATOM	2265	N	TRP	421	46.870	37.556	42.490	1.00	18.99	BTKB
ATOM	2266	CA	TRP	421	46.184	38.800	42.789	1.00	19.16	BTKB
ATOM	2267	CB	TRP	421	44.683	38.548	42.875	1.00	21.71	BTKB
ATOM	2268	CG	TRP	421	43.869	39.797	42.944	1.00	23.50	BTKB
ATOM	2269	CD2	TRP	421	42.920	40.148	43.959	1.00	22.38	BTKB
ATOM	2270	CE2	TRP	421	42.370	41.394	43.599	1.00	25.22	BTKB
ATOM	2271	CE3	TRP	421	42.482	39.528	45.137	1.00	26.12	BTKB
ATOM	2272	CD1	TRP	421	43.859	40.817	42.041	1.00	21.67	BTKB
ATOM	2273	NE1	TRP	421	42.962	41.778	42.425	1.00	26.88	BTKB
ATOM	2274	CZ2	TRP	421	41.402	42.036	44.372	1.00	26.92	BTKB
ATOM	2275	CZ3	TRP	421	41.521	40.166	45.907	1.00	27.03	BTKB
ATOM	2276	CH2	TRP	421	40.991	41.408	45.520	1.00	26.73	BTKB
ATOM	2277	C	TRP	421	46.694	39.348	44.114	1.00	20.06	BTKB
ATOM	2278	O	TRP	421	46.905	38.587	45.059	1.00	21.40	BTKB
ATOM	2279	N	ARG	422	46.907	40.664	44.166	1.00	22.24	BTKB
ATOM	2280	CA	ARG	422	47.394	41.358	45.366	1.00	24.43	BTKB
ATOM	2281	CB	ARG	422	46.387	41.228	46.520	1.00	25.85	BTKB
ATOM	2282	CG	ARG	422	44.960	41.672	46.222	1.00	27.33	BTKB
ATOM	2283	CD	ARG	422	44.832	43.176	46.095	1.00	29.62	BTKB
ATOM	2284	NE	ARG	422	43.473	43.622	46.388	1.00	29.09	BTKB
ATOM	2285	CZ	ARG	422	42.944	43.659	47.607	1.00	28.92	BTKB
ATOM	2286	NH1	ARG	422	41.698	44.078	47.781	1.00	31.54	BTKB
ATOM	2287	NH2	ARG	422	43.654	43.273	48.657	1.00	31.57	BTKB
ATOM	2288	C	ARG	422	48.761	40.854	45.841	1.00	26.12	BTKB
ATOM	2289	O	ARG	422	49.068	40.896	47.033	1.00	24.76	BTKB
ATOM	2290	N	GLY	423	49.551	40.328	44.911	1.00	27.65	BTKB
ATOM	2291	CA	GLY	423	50.879	39.826	45.235	1.00	27.28	BTKB
ATOM	2292	C	GLY	423	50.970	38.814	46.366	1.00	28.60	BTKB
ATOM	2293	O	GLY	423	52.057	38.569	46.892	1.00	28.45	BTKB
ATOM	2294	N	ALA	424	49.848	38.200	46.724	1.00	29.60	BTKB
ATOM	2295	CA	ALA	424	49.841	37.216	47.800	1.00	27.82	BTKB
ATOM	2296	CB	ALA	424	49.602	37.902	49.142	1.00	30.88	BTKB
ATOM	2297	C	ALA	424	48.807	36.124	47.584	1.00	25.78	BTKB
ATOM	2298	O	ALA	424	48.987	35.002	48.047	1.00	25.99	BTKB
ATOM	2299	N	ALA	425	47.739	36.442	46.862	1.00	24.03	BTKB
ATOM	2300	CA	ALA	425	46.677	35.476	46.604	1.00	24.48	BTKB
ATOM	2301	CB	ALA	425	45.313	36.151	46.782	1.00	20.10	BTKB
ATOM	2302	C	ALA	425	46.762	34.806	45.227	1.00	23.85	BTKB
ATOM	2303	O	ALA	425	46.766	35.479	44.194	1.00	23.75	BTKB
ATOM	2304	N	ASP	426	46.863	33.481	45.214	1.00	23.12	BTKB
ATOM	2305	CA	ASP	426	46.907	32.739	43.955	1.00	22.00	BTKB
ATOM	2306	CB	ASP	426	47.540	31.360	44.162	1.00	27.54	BTKB
ATOM	2307	CG	ASP	426	49.016	31.443	44.531	1.00	28.92	BTKB
ATOM	2308	OD1	ASP	426	49.596	30.404	44.915	1.00	30.24	BTKB
ATOM	2309	OD2	ASP	426	49.600	32.544	44.435	1.00	28.52	BTKB
ATOM	2310	C	ASP	426	45.469	32.615	43.458	1.00	17.08	BTKB
ATOM	2311	O	ASP	426	44.567	32.310	44.237	1.00	15.85	BTKB
ATOM	2312	N	VAL	427	45.255	32.841	42.166	1.00	13.56	BTKB
ATOM	2313	CA	VAL	427	43.909	32.810	41.603	1.00	12.45	BTKB

	Atom Number	Atom Type	Amino Acid Residue		X	Y	Z	Occ.	Temp Factor	
ATOM	2314	CB	VAL	427	43.340	34.246	41.418	1.00	10.01	BTKB
ATOM	2315	CG1	VAL	427	43.282	34.991	42.741	1.00	12.17	BTKB
ATOM	2316	CG2	VAL	427	44.184	35.015	40.409	1.00	12.71	BTKB
ATOM	2317	C	VAL	427	43.767	32.131	40.246	1.00	13.93	BTKB
ATOM	2318	O	VAL	427	44.742	31.905	39.528	1.00	15.85	BTKB
ATOM	2319	N	ALA	428	42.517	31.853	39.898	1.00	12.30	BTKB
ATOM	2320	CA	ALA	428	42.152	31.245	38.631	1.00	12.30	BTKB
ATOM	2321	CB	ALA	428	41.386	29.957	38.871	1.00	10.91	BTKB
ATOM	2322	C	ALA	428	41.238	32.288	38.023	1.00	10.93	BTKB
ATOM	2323	O	ALA	428	40.383	32.823	38.724	1.00	12.65	BTKB
ATOM	2324	N	ILE	429	41.436	32.618	36.750	1.00	12.14	BTKB
ATOM	2325	CA	ILE	429	40.597	33.622	36.110	1.00	14.63	BTKB
ATOM	2326	CB	ILE	429	41.441	34.832	35.525	1.00	13.45	BTKB
ATOM	2327	CG2	ILE	429	42.825	34.396	35.083	1.00	15.33	BTKB
ATOM	2328	CG1	ILE	429	40.693	35.558	34.415	1.00	7.39	BTKB
ATOM	2329	CD	ILE	429	40.969	35.023	33.036	1.00	16.26	BTKB
ATOM	2330	C	ILE	429	39.573	33.051	35.124	1.00	18.66	BTKB
ATOM	2331	O	ILE	429	39.934	32.469	34.095	1.00	19.46	BTKB
ATOM	2332	N	LYS	430	38.295	33.199	35.482	1.00	19.80	BTKB
ATOM	2333	CA	LYS	430	37.161	32.726	34.689	1.00	21.31	BTKB
ATOM	2334	CB	LYS	430	35.978	32.421	35.606	1.00	20.55	BTKB
ATOM	2335	CG	LYS	430	34.755	31.868	34.901	1.00	25.20	BTKB
ATOM	2336	CD	LYS	430	34.992	30.445	34.442	1.00	29.40	BTKB
ATOM	2337	CE	LYS	430	33.692	29.770	34.064	1.00	29.23	BTKB
ATOM	2338	NZ	LYS	430	32.682	29.854	35.162	1.00	33.94	BTKB
ATOM	2339	C	LYS	430	36.749	33.769	33.650	1.00	21.71	BTKB
ATOM	2340	O	LYS	430	36.214	34.820	33.994	1.00	17.94	BTKB
ATOM	2341	N	MET	431	36.968	33.438	32.382	1.00	24.22	BTKB
ATOM	2342	CA	MET	431	36.668	34.320	31.260	1.00	26.94	BTKB
ATOM	2343	CB	MET	431	37.814	34.211	30.257	1.00	29.16	BTKB
ATOM	2344	CG	MET	431	37.670	35.004	28.993	1.00	28.32	BTKB
ATOM	2345	SD	MET	431	38.671	34.218	27.732	1.00	29.24	BTKB
ATOM	2346	CE	MET	431	37.422	33.825	26.504	1.00	30.72	BTKB
ATOM	2347	C	MET	431	35.339	33.992	30.575	1.00	30.22	BTKB
ATOM	2348	O	MET	431	34.966	32.823	30.447	1.00	32.27	BTKB
ATOM	2349	N	ILE	432	34.632	35.031	30.129	1.00	34.07	BTKB
ATOM	2350	CA	ILE	432	33.343	34.858	29.452	1.00	35.28	BTKB
ATOM	2351	CB	ILE	432	32.218	35.740	30.089	1.00	34.75	BTKB
ATOM	2352	CG2	ILE	432	30.852	35.123	29.802	1.00	33.26	BTKB
ATOM	2353	CG1	ILE	432	32.396	35.858	31.606	1.00	33.83	BTKB
ATOM	2354	CD	ILE	432	32.347	34.538	32.352	1.00	35.34	BTKB
ATOM	2355	C	ILE	432	33.499	35.208	27.964	1.00	33.87	BTKB
ATOM	2356	O	ILE	432	34.414	34.717	27.309	1.00	34.55	BTKB
ATOM	2357	N	LYS	433	32.623	36.067	27.445	1.00	33.43	BTKB
ATOM	2358	CA	LYS	433	32.646	36.499	26.045	1.00	31.18	BTKB
ATOM	2359	CB	LYS	433	31.888	35.507	25.146	1.00	27.65	BTKB
ATOM	2360	CG	LYS	433	32.416	34.073	25.107	1.00	24.55	BTKB
ATOM	2361	CD	LYS	433	33.793	33.983	24.475	1.00	27.10	BTKB
ATOM	2362	CE	LYS	433	33.807	34.598	23.094	1.00	24.68	BTKB
ATOM	2363	NZ	LYS	433	35.145	34.557	22.439	1.00	18.58	BTKB
ATOM	2364	C	LYS	433	31.910	37.837	25.985	1.00	30.74	BTKB
ATOM	2365	O	LYS	433	30.782	37.944	26.483	1.00	29.85	BTKB
ATOM	2366	N	GLU	434	32.535	38.861	25.410	1.00	30.55	BTKB
ATOM	2367	CA	GLU	434	31.863	40.153	25.300	1.00	29.48	BTKB
ATOM	2368	CB	GLU	434	32.850	41.282	24.994	1.00	29.95	BTKB
ATOM	2369	CG	GLU	434	32.215	42.691	24.991	1.00	26.07	BTKB
ATOM	2370	CD	GLU	434	33.233	43.829	24.915	1.00	21.62	BTKB
ATOM	2371	OE1	GLU	434	34.425	43.574	24.649	1.00	24.27	BTKB

	Atom Number	Atom Type	Amino Acid Residue		X	Y	Z	Occ.	Temp Factor	
ATOM	2372	OE2	GLU	434	32.837	44.992	25.130	1.00	19.02	BTKB
ATOM	2373	C	GLU	434	30.835	40.005	24.189	1.00	31.41	BTKB
ATOM	2374	O	GLU	434	31.047	40.420	23.054	1.00	29.99	BTKB
ATOM	2375	N	GLY	435	29.742	39.334	24.526	1.00	35.03	BTKB
ATOM	2376	CA	GLY	435	28.671	39.085	23.581	1.00	37.48	BTKB
ATOM	2377	C	GLY	435	27.610	38.249	24.270	1.00	39.46	BTKB
ATOM	2378	O	GLY	435	26.795	37.605	23.613	1.00	40.93	BTKB
ATOM	2379	N	SER	436	27.626	38.257	25.603	1.00	37.43	BTKB
ATOM	2380	CA	SER	436	26.671	37.497	26.392	1.00	37.99	BTKB
ATOM	2381	CB	SER	436	27.107	36.030	26.476	1.00	41.23	BTKB
ATOM	2382	OG	SER	436	27.624	35.565	25.240	1.00	42.60	BTKB
ATOM	2383	C	SER	436	26.560	38.083	27.799	1.00	39.64	BTKB
ATOM	2384	O	SER	436	25.600	38.789	28.110	1.00	41.69	BTKB
ATOM	2385	N	MET	437	27.555	37.798	28.640	1.00	39.73	BTKB
ATOM	2386	CA	MET	437	27.580	38.277	30.024	1.00	38.94	BTKB
ATOM	2387	CB	MET	437	28.591	37.462	30.832	1.00	40.22	BTKB
ATOM	2388	CG	MET	437	28.318	37.367	32.325	1.00	35.33	BTKB
ATOM	2389	SD	MET	437	29.214	35.957	33.007	1.00	41.10	BTKB
ATOM	2390	CE	MET	437	29.769	36.561	34.621	1.00	31.14	BTKB
ATOM	2391	C	MET	437	27.923	39.767	30.095	1.00	39.09	BTKB
ATOM	2392	O	MET	437	28.389	40.353	29.114	1.00	36.63	BTKB
ATOM	2393	N	SER	438	27.723	40.367	31.267	1.00	39.27	BTKB
ATOM	2394	CA	SER	438	27.990	41.787	31.447	1.00	37.97	BTKB
ATOM	2395	CB	SER	438	26.845	42.593	30.835	1.00	38.54	BTKB
ATOM	2396	OG	SER	438	25.603	42.171	31.372	1.00	33.86	BTKB
ATOM	2397	C	SER	438	28.150	42.199	32.906	1.00	36.36	BTKB
ATOM	2398	O	SER	438	27.639	41.529	33.805	1.00	34.72	BTKB
ATOM	2399	N	GLU	439	28.807	43.339	33.117	1.00	37.58	BTKB
ATOM	2400	CA	GLU	439	29.034	43.904	34.452	1.00	37.09	BTKB
ATOM	2401	CB	GLU	439	29.945	45.139	34.361	1.00	37.29	BTKB
ATOM	2402	CG	GLU	439	29.372	46.302	33.537	1.00	37.02	BTKB
ATOM	2403	CD	GLU	439	30.217	47.572	33.606	1.00	36.40	BTKB
ATOM	2404	OE1	GLU	439	30.640	47.957	34.719	1.00	36.07	BTKB
ATOM	2405	OE2	GLU	439	30.450	48.195	32.544	1.00	35.38	BTKB
ATOM	2406	C	GLU	439	27.728	44.309	35.146	1.00	36.76	BTKB
ATOM	2407	O	GLU	439	27.696	44.522	36.363	1.00	32.43	BTKB
ATOM	2408	N	ASP	440	26.662	44.426	34.359	1.00	35.30	BTKB
ATOM	2409	CA	ASP	440	25.362	44.826	34.867	1.00	32.48	BTKB
ATOM	2410	CB	ASP	440	24.662	45.730	33.848	1.00	36.16	BTKB
ATOM	2411	CG	ASP	440	25.592	46.775	33.253	1.00	40.98	BTKB
ATOM	2412	OD1	ASP	440	25.560	47.945	33.691	1.00	39.71	BTKB
ATOM	2413	OD2	ASP	440	26.358	46.426	32.334	1.00	37.76	BTKB
ATOM	2414	C	ASP	440	24.480	43.626	35.179	1.00	31.97	BTKB
ATOM	2415	O	ASP	440	23.521	43.745	35.943	1.00	28.02	BTKB
ATOM	2416	N	GLU	441	24.783	42.477	34.574	1.00	33.36	BTKB
ATOM	2417	CA	GLU	441	23.978	41.278	34.815	1.00	33.34	BTKB
ATOM	2418	CB	GLU	441	24.000	40.317	33.601	1.00	33.19	BTKB
ATOM	2419	CG	GLU	441	25.090	39.216	33.599	1.00	34.36	BTKB
ATOM	2420	CD	GLU	441	24.702	37.934	34.361	1.00	36.00	BTKB
ATOM	2421	OE1	GLU	441	25.523	36.989	34.398	1.00	35.37	BTKB
ATOM	2422	OE2	GLU	441	23.585	37.858	34.918	1.00	34.93	BTKB
ATOM	2423	C	GLU	441	24.414	40.546	36.077	1.00	32.17	BTKB
ATOM	2424	O	GLU	441	23.586	40.191	36.930	1.00	29.45	BTKB
ATOM	2425	N	PHE	442	25.719	40.357	36.220	1.00	29.54	BTKB
ATOM	2426	CA	PHE	442	26.202	39.631	37.366	1.00	31.35	BTKB
ATOM	2427	CB	PHE	442	27.382	38.730	36.988	1.00	28.63	BTKB
ATOM	2428	CG	PHE	442	28.708	39.424	36.944	1.00	22.65	BTKB
ATOM	2429	CD1	PHE	442	29.837	38.790	37.440	1.00	20.14	BTKB

	Atom Number	Atom Type	Amino Acid Residue		X	Y	Z	Occ.	Temp Factor	
ATOM	2430	CD2	PHE	442	28.843	40.683	36.387	1.00	22.28	BTKB
ATOM	2431	CE1	PHE	442	31.072	39.390	37.379	1.00	17.92	BTKB
ATOM	2432	CE2	PHE	442	30.081	41.291	36.323	1.00	24.89	BTKB
ATOM	2433	CZ	PHE	442	31.198	40.641	36.822	1.00	18.41	BTKB
ATOM	2434	C	PHE	442	26.494	40.449	38.604	1.00	32.00	BTKB
ATOM	2435	O	PHE	442	26.809	39.879	39.634	1.00	34.02	BTKB
ATOM	2436	N	ILE	443	26.343	41.767	38.529	1.00	31.37	BTKB
ATOM	2437	CA	ILE	443	26.608	42.613	39.689	1.00	34.20	BTKB
ATOM	2438	CB	ILE	443	26.334	44.114	39.393	1.00	35.12	BTKB
ATOM	2439	CG2	ILE	443	24.913	44.314	38.889	1.00	35.43	BTKB
ATOM	2440	CG1	ILE	443	26.577	44.961	40.649	1.00	36.71	BTKB
ATOM	2441	CD	ILE	443	28.010	44.938	41.152	1.00	33.98	BTKB
ATOM	2442	C	ILE	443	25.758	42.142	40.866	1.00	34.50	BTKB
ATOM	2443	O	ILE	443	26.243	42.006	41.993	1.00	33.00	BTKB
ATOM	2444	N	GLU	444	24.499	41.840	40.577	1.00	33.96	BTKB
ATOM	2445	CA	GLU	444	23.576	41.364	41.593	1.00	33.66	BTKB
ATOM	2446	CB	GLU	444	22.199	41.122	40.955	1.00	34.83	BTKB
ATOM	2447	CG	GLU	444	21.019	41.072	41.920	1.00	34.28	BTKB
ATOM	2448	CD	GLU	444	20.937	39.782	42.712	1.00	35.97	BTKB
ATOM	2449	OE1	GLU	444	21.288	38.710	42.167	1.00	32.68	BTKB
ATOM	2450	OE2	GLU	444	20.501	39.841	43.881	1.00	36.01	BTKB
ATOM	2451	C	GLU	444	24.159	40.064	42.158	1.00	33.11	BTKB
ATOM	2452	O	GLU	444	24.610	40.024	43.305	1.00	30.69	BTKB
ATOM	2453	N	GLU	445	24.239	39.042	41.307	1.00	32.60	BTKB
ATOM	2454	CA	GLU	445	24.752	37.731	41.688	1.00	30.53	BTKB
ATOM	2455	CB	GLU	445	24.753	36.784	40.486	1.00	31.01	BTKB
ATOM	2456	CG	GLU	445	23.366	36.338	40.032	1.00	28.32	BTKB
ATOM	2457	CD	GLU	445	23.382	35.007	39.296	1.00	28.84	BTKB
ATOM	2458	OE1	GLU	445	24.392	34.275	39.386	1.00	28.01	BTKB
ATOM	2459	OE2	GLU	445	22.372	34.682	38.640	1.00	27.39	BTKB
ATOM	2460	C	GLU	445	26.134	37.732	42.328	1.00	31.12	BTKB
ATOM	2461	O	GLU	445	26.404	36.934	43.225	1.00	33.61	BTKB
ATOM	2462	N	ALA	446	26.993	38.643	41.888	1.00	30.01	BTKB
ATOM	2463	CA	ALA	446	28.351	38.739	42.410	1.00	29.17	BTKB
ATOM	2464	CB	ALA	446	29.145	39.800	41.655	1.00	27.22	BTKB
ATOM	2465	C	ALA	446	28.312	39.065	43.894	1.00	30.07	BTKB
ATOM	2466	O	ALA	446	28.845	38.317	44.712	1.00	31.57	BTKB
ATOM	2467	N	LYS	447	27.634	40.153	44.240	1.00	30.54	BTKB
ATOM	2468	CA	LYS	447	27.525	40.574	45.631	1.00	29.93	BTKB
ATOM	2469	CB	LYS	447	26.676	41.847	45.742	1.00	29.51	BTKB
ATOM	2470	CG	LYS	447	27.176	43.023	44.906	1.00	27.76	BTKB
ATOM	2471	CD	LYS	447	28.634	43.362	45.198	1.00	24.63	BTKB
ATOM	2472	CE	LYS	447	28.846	43.812	46.635	1.00	23.47	BTKB
ATOM	2473	NZ	LYS	447	30.298	43.984	46.929	1.00	24.76	BTKB
ATOM	2474	C	LYS	447	26.917	39.465	46.487	1.00	31.89	BTKB
ATOM	2475	O	LYS	447	27.393	39.194	47.597	1.00	31.20	BTKB
ATOM	2476	N	VAL	448	25.893	38.804	45.949	1.00	31.29	BTKB
ATOM	2477	CA	VAL	448	25.207	37.725	46.651	1.00	30.04	BTKB
ATOM	2478	CB	VAL	448	23.958	37.250	45.882	1.00	29.87	BTKB
ATOM	2479	CG1	VAL	448	23.189	36.226	46.705	1.00	28.85	BTKB
ATOM	2480	CG2	VAL	448	23.062	38.428	45.547	1.00	33.30	BTKB
ATOM	2481	C	VAL	448	26.126	36.531	46.881	1.00	30.34	BTKB
ATOM	2482	O	VAL	448	26.074	35.900	47.939	1.00	31.49	BTKB
ATOM	2483	N	MET	449	26.963	36.215	45.897	1.00	29.17	BTKB
ATOM	2484	CA	MET	449	27.882	35.091	46.027	1.00	27.85	BTKB
ATOM	2485	CB	MET	449	28.473	34.708	44.676	1.00	27.95	BTKB
ATOM	2486	CG	MET	449	27.570	33.842	43.834	1.00	25.86	BTKB
ATOM	2487	SD	MET	449	27.991	33.992	42.101	1.00	28.55	BTKB

	Atom Number	Atom Type	Amino Acid Residue		X	Y	Z	Occ.	Temp Factor	
ATOM	2488	CE	MET	449	29.603	33.105	42.046	1.00	24.75	BTKB
ATOM	2489	C	MET	449	28.994	35.425	46.997	1.00	29.13	BTKB
ATOM	2490	O	MET	449	29.497	34.551	47.694	1.00	32.51	BTKB
ATOM	2491	N	MET	450	29.376	36.696	47.046	1.00	27.71	BTKB
ATOM	2492	CA	MET	450	30.422	37.130	47.955	1.00	25.39	BTKB
ATOM	2493	CB	MET	450	30.926	38.512	47.558	1.00	24.26	BTKB
ATOM	2494	CG	MET	450	31.553	38.506	46.179	1.00	23.94	BTKB
ATOM	2495	SD	MET	450	32.473	39.970	45.741	1.00	32.01	BTKB
ATOM	2496	CE	MET	450	33.957	39.761	46.735	1.00	25.95	BTKB
ATOM	2497	C	MET	450	29.883	37.103	49.381	1.00	27.55	BTKB
ATOM	2498	O	MET	450	30.627	37.257	50.351	1.00	28.08	BTKB
ATOM	2499	N	ASN	451	28.573	36.904	49.499	1.00	24.81	BTKB
ATOM	2500	CA	ASN	451	27.919	36.800	50.796	1.00	23.63	BTKB
ATOM	2501	CB	ASN	451	26.414	37.017	50.662	1.00	22.42	BTKB
ATOM	2502	CG	ASN	451	25.999	38.446	50.915	1.00	20.08	BTKB
ATOM	2503	OD1	ASN	451	24.868	38.701	51.326	1.00	22.32	BTKB
ATOM	2504	ND2	ASN	451	26.896	39.390	50.656	1.00	17.73	BTKB
ATOM	2505	C	ASN	451	28.157	35.389	51.299	1.00	24.31	BTKB
ATOM	2506	O	ASN	451	27.841	35.065	52.447	1.00	23.55	BTKB
ATOM	2507	N	LEU	452	28.657	34.539	50.406	1.00	23.43	BTKB
ATOM	2508	CA	LEU	452	28.946	33.146	50.714	1.00	21.56	BTKB
ATOM	2509	CB	LEU	452	28.585	32.255	49.522	1.00	21.06	BTKB
ATOM	2510	CG	LEU	452	27.138	31.762	49.400	1.00	20.32	BTKB
ATOM	2511	CD1	LEU	452	26.150	32.810	49.869	1.00	20.52	BTKB
ATOM	2512	CD2	LEU	452	26.869	31.351	47.968	1.00	18.22	BTKB
ATOM	2513	C	LEU	452	30.414	32.985	51.050	1.00	22.10	BTKB
ATOM	2514	O	LEU	452	31.280	33.131	50.191	1.00	25.35	BTKB
ATOM	2515	N	SER	453	30.688	32.718	52.317	1.00	22.10	BTKB
ATOM	2516	CA	SER	453	32.047	32.525	52.784	1.00	21.51	BTKB
ATOM	2517	CB	SER	453	32.537	33.751	53.565	1.00	27.28	BTKB
ATOM	2518	OG	SER	453	32.794	34.849	52.707	1.00	32.08	BTKB
ATOM	2519	C	SER	453	32.051	31.314	53.690	1.00	20.26	BTKB
ATOM	2520	O	SER	453	31.201	31.182	54.576	1.00	21.49	BTKB
ATOM	2521	N	HIS	454	32.979	30.407	53.425	1.00	16.43	BTKB
ATOM	2522	CA	HIS	454	33.134	29.195	54.203	1.00	14.23	BTKB
ATOM	2523	CB	HIS	454	31.930	28.256	54.025	1.00	13.19	BTKB
ATOM	2524	CG	HIS	454	31.921	27.100	54.982	1.00	12.78	BTKB
ATOM	2525	CD2	HIS	454	32.496	25.875	54.910	1.00	11.15	BTKB
ATOM	2526	ND1	HIS	454	31.317	27.164	56.218	1.00	13.51	BTKB
ATOM	2527	CE1	HIS	454	31.526	26.033	56.871	1.00	12.23	BTKB
ATOM	2528	NE2	HIS	454	32.241	25.235	56.099	1.00	6.57	BTKB
ATOM	2529	C	HIS	454	34.378	28.535	53.666	1.00	13.02	BTKB
ATOM	2530	O	HIS	454	34.569	28.478	52.462	1.00	14.69	BTKB
ATOM	2531	N	GLU	455	35.225	28.064	54.572	1.00	17.21	BTKB
ATOM	2532	CA	GLU	455	36.472	27.373	54.247	1.00	19.94	BTKB
ATOM	2533	CB	GLU	455	37.152	26.954	55.569	1.00	25.60	BTKB
ATOM	2534	CG	GLU	455	37.914	25.623	55.594	1.00	26.02	BTKB
ATOM	2535	CD	GLU	455	39.213	25.637	54.816	1.00	23.62	BTKB
ATOM	2536	OE1	GLU	455	39.525	24.609	54.188	1.00	26.91	BTKB
ATOM	2537	OE2	GLU	455	39.926	26.661	54.834	1.00	26.89	BTKB
ATOM	2538	C	GLU	455	36.294	26.179	53.294	1.00	18.16	BTKB
ATOM	2539	O	GLU	455	37.260	25.701	52.706	1.00	17.46	BTKB
ATOM	2540	N	LYS	456	35.059	25.716	53.121	1.00	17.18	BTKB
ATOM	2541	CA	LYS	456	34.791	24.581	52.239	1.00	15.92	BTKB
ATOM	2542	CB	LYS	456	33.958	23.528	52.970	1.00	18.08	BTKB
ATOM	2543	CG	LYS	456	34.661	22.920	54.182	1.00	15.32	BTKB
ATOM	2544	CD	LYS	456	35.909	22.160	53.764	1.00	16.08	BTKB
ATOM	2545	CE	LYS	456	36.628	21.511	54.935	1.00	14.75	BTKB

Atom Number	Atom Type	Amino Acid Residue		X	Y	Z	Occ.	Temp Factor	
ATOM 2546	NZ	LYS	456	37.413	22.460	55.750	1.00	15.29	BTKB
ATOM 2547	C	LYS	456	34.148	24.962	50.897	1.00	16.33	BTKB
ATOM 2548	O	LYS	456	33.760	24.091	50.108	1.00	11.16	BTKB
ATOM 2549	N	LEU	457	34.015	26.265	50.653	1.00	15.73	BTKB
ATOM 2550	CA	LEU	457	33.454	26.774	49.404	1.00	14.51	BTKB
ATOM 2551	CB	LEU	457	32.349	27.809	49.658	1.00	14.58	BTKB
ATOM 2552	CG	LEU	457	30.948	27.463	50.169	1.00	11.43	BTKB
ATOM 2553	CD1	LEU	457	30.166	28.752	50.355	1.00	9.22	BTKB
ATOM 2554	CD2	LEU	457	30.216	26.576	49.186	1.00	13.55	BTKB
ATOM 2555	C	LEU	457	34.613	27.473	48.722	1.00	11.29	BTKB
ATOM 2556	O	LEU	457	35.400	28.152	49.385	1.00	14.89	BTKB
ATOM 2557	N	VAL	458	34.756	27.282	47.417	1.00	14.60	BTKB
ATOM 2558	CA	VAL	458	35.831	27.945	46.690	1.00	13.47	BTKB
ATOM 2559	CB	VAL	458	36.015	27.338	45.292	1.00	10.95	BTKB
ATOM 2560	CG1	VAL	458	37.107	28.080	44.523	1.00	8.36	BTKB
ATOM 2561	CG2	VAL	458	36.377	25.870	45.425	1.00	4.94	BTKB
ATOM 2562	C	VAL	458	35.418	29.414	46.627	1.00	17.55	BTKB
ATOM 2563	O	VAL	458	34.339	29.744	46.129	1.00	19.50	BTKB
ATOM 2564	N	GLN	459	36.256	30.288	47.173	1.00	19.70	BTKB
ATOM 2565	CA	GLN	459	35.930	31.710	47.231	1.00	22.06	BTKB
ATOM 2566	CB	GLN	459	36.572	32.360	48.461	1.00	22.66	BTKB
ATOM 2567	CG	GLN	459	38.082	32.441	48.427	1.00	29.48	BTKB
ATOM 2568	CD	GLN	459	38.657	32.969	49.727	1.00	31.10	BTKB
ATOM 2569	OE1	GLN	459	39.341	32.248	50.454	1.00	26.32	BTKB
ATOM 2570	NE2	GLN	459	38.370	34.230	50.033	1.00	29.38	BTKB
ATOM 2571	C	GLN	459	36.165	32.594	46.019	1.00	21.06	BTKB
ATOM 2572	O	GLN	459	37.209	32.543	45.370	1.00	22.08	BTKB
ATOM 2573	N	LEU	460	35.177	33.435	45.754	1.00	21.47	BTKB
ATOM 2574	CA	LEU	460	35.224	34.395	44.665	1.00	23.95	BTKB
ATOM 2575	CB	LEU	460	33.786	34.778	44.269	1.00	22.50	BTKB
ATOM 2576	CG	LEU	460	33.466	35.635	43.034	1.00	22.00	BTKB
ATOM 2577	CD1	LEU	460	31.973	35.572	42.746	1.00	24.79	BTKB
ATOM 2578	CD2	LEU	460	33.895	37.074	43.243	1.00	22.74	BTKB
ATOM 2579	C	LEU	460	35.953	35.592	45.278	1.00	24.95	BTKB
ATOM 2580	O	LEU	460	35.416	36.254	46.165	1.00	25.13	BTKB
ATOM 2581	N	TYR	461	37.198	35.821	44.873	1.00	24.81	BTKB
ATOM 2582	CA	TYR	461	37.966	36.943	45.411	1.00	25.17	BTKB
ATOM 2583	CB	TYR	461	39.457	36.816	45.064	1.00	25.82	BTKB
ATOM 2584	CG	TYR	461	40.199	35.689	45.774	1.00	25.50	BTKB
ATOM 2585	CD1	TYR	461	40.773	34.643	45.050	1.00	26.73	BTKB
ATOM 2586	CE1	TYR	461	41.476	33.618	45.682	1.00	24.71	BTKB
ATOM 2587	CD2	TYR	461	40.347	35.682	47.161	1.00	25.96	BTKB
ATOM 2588	CE2	TYR	461	41.050	34.659	47.807	1.00	25.37	BTKB
ATOM 2589	CZ	TYR	461	41.612	33.631	47.058	1.00	25.30	BTKB
ATOM 2590	OH	TYR	461	42.317	32.622	47.681	1.00	25.28	BTKB
ATOM 2591	C	TYR	461	37.407	38.259	44.871	1.00	27.25	BTKB
ATOM 2592	O	TYR	461	37.293	39.246	45.596	1.00	26.29	BTKB
ATOM 2593	N	GLY	462	37.041	38.262	43.596	1.00	27.06	BTKB
ATOM 2594	CA	GLY	462	36.499	39.464	42.993	1.00	24.45	BTKB
ATOM 2595	C	GLY	462	36.196	39.275	41.523	1.00	22.73	BTKB
ATOM 2596	O	GLY	462	36.553	38.262	40.935	1.00	20.21	BTKB
ATOM 2597	N	VAL	463	35.527	40.253	40.930	1.00	24.33	BTKB
ATOM 2598	CA	VAL	463	35.182	40.198	39.523	1.00	24.62	BTKB
ATOM 2599	CB	VAL	463	33.697	39.891	39.319	1.00	27.36	BTKB
ATOM 2600	CG1	VAL	463	33.368	38.519	39.854	1.00	33.31	BTKB
ATOM 2601	CG2	VAL	463	32.843	40.935	40.011	1.00	30.70	BTKB
ATOM 2602	C	VAL	463	35.478	41.528	38.861	1.00	24.47	BTKB
ATOM 2603	O	VAL	463	35.418	42.584	39.504	1.00	24.70	BTKB

	Atom Number	Atom Type	Amino Acid Residue		X	Y	Z	Occ.	Temp Factor	
ATOM	2604	N	CYS	464	35.829	41.473	37.584	1.00	27.38	BTKB
ATOM	2605	CA	CYS	464	36.115	42.677	36.828	1.00	29.15	BTKB
ATOM	2606	CB	CYS	464	37.073	42.384	35.675	1.00	33.36	BTKB
ATOM	2607	SG	CYS	464	37.677	43.868	34.853	1.00	38.92	BTKB
ATOM	2608	C	CYS	464	34.779	43.162	36.302	1.00	29.60	BTKB
ATOM	2609	O	CYS	464	34.321	42.744	35.238	1.00	27.69	BTKB
ATOM	2610	N	THR	465	34.113	43.960	37.125	1.00	31.56	BTKB
ATOM	2611	CA	THR	465	32.815	44.528	36.807	1.00	30.98	BTKB
ATOM	2612	CB	THR	465	32.208	45.184	38.058	1.00	31.96	BTKB
ATOM	2613	OG1	THR	465	33.219	45.959	38.723	1.00	30.73	BTKB
ATOM	2614	CG2	THR	465	31.652	44.127	39.010	1.00	33.13	BTKB
ATOM	2615	C	THR	465	32.982	45.582	35.731	1.00	31.69	BTKB
ATOM	2616	O	THR	465	32.916	46.778	36.016	1.00	33.93	BTKB
ATOM	2617	N	LYS	466	33.238	45.138	34.508	1.00	32.07	BTKB
ATOM	2618	CA	LYS	466	33.420	46.040	33.379	1.00	31.90	BTKB
ATOM	2619	CB	LYS	466	34.908	46.348	33.185	1.00	29.79	BTKB
ATOM	2620	CG	LYS	466	35.199	47.726	32.597	1.00	28.18	BTKB
ATOM	2621	CD	LYS	466	34.692	48.854	33.507	1.00	28.96	BTKB
ATOM	2622	CE	LYS	466	33.405	49.481	32.968	1.00	30.68	BTKB
ATOM	2623	NZ	LYS	466	32.784	50.444	33.929	1.00	29.32	BTKB
ATOM	2624	C	LYS	466	32.844	45.326	32.162	1.00	35.07	BTKB
ATOM	2625	O	LYS	466	32.073	44.374	32.314	1.00	35.06	BTKB
ATOM	2626	N	GLN	467	33.184	45.770	30.956	1.00	39.06	BTKB
ATOM	2627	CA	GLN	467	32.647	45.103	29.782	1.00	40.26	BTKB
ATOM	2628	CB	GLN	467	31.613	45.967	29.057	1.00	40.39	BTKB
ATOM	2629	CG	GLN	467	30.831	45.184	28.005	1.00	39.46	BTKB
ATOM	2630	CD	GLN	467	30.526	43.757	28.451	1.00	38.12	BTKB
ATOM	2631	OE1	GLN	467	31.174	42.807	28.017	1.00	31.06	BTKB
ATOM	2632	NE2	GLN	467	29.560	43.608	29.344	1.00	37.49	BTKB
ATOM	2633	C	GLN	467	33.672	44.568	28.805	1.00	40.30	BTKB
ATOM	2634	O	GLN	467	34.461	45.314	28.224	1.00	41.34	BTKB
ATOM	2635	N	ARG	468	33.591	43.255	28.632	1.00	40.07	BTKB
ATOM	2636	CA	ARG	468	34.420	42.419	27.765	1.00	39.22	BTKB
ATOM	2637	CB	ARG	468	35.865	42.938	27.661	1.00	38.37	BTKB
ATOM	2638	CG	ARG	468	36.689	42.820	28.929	1.00	37.01	BTKB
ATOM	2639	CD	ARG	468	38.159	43.070	28.635	1.00	34.26	BTKB
ATOM	2640	NE	ARG	468	38.710	42.100	27.691	1.00	30.22	BTKB
ATOM	2641	CZ	ARG	468	38.997	40.835	27.989	1.00	33.17	BTKB
ATOM	2642	NH1	ARG	468	38.778	40.370	29.209	1.00	34.06	BTKB
ATOM	2643	NH2	ARG	468	39.537	40.043	27.073	1.00	32.25	BTKB
ATOM	2644	C	ARG	468	34.370	41.078	28.502	1.00	38.55	BTKB
ATOM	2645	O	ARG	468	33.602	40.937	29.462	1.00	40.13	BTKB
ATOM	2646	N	PRO	469	35.103	40.049	28.027	1.00	36.71	BTKB
ATOM	2647	CD	PRO	469	35.916	39.864	26.809	1.00	34.66	BTKB
ATOM	2648	CA	PRO	469	35.012	38.803	28.792	1.00	34.01	BTKB
ATOM	2649	CB	PRO	469	36.128	37.964	28.182	1.00	32.71	BTKB
ATOM	2650	CG	PRO	469	36.058	38.358	26.734	1.00	32.30	BTKB
ATOM	2651	C	PRO	469	35.277	39.133	30.259	1.00	34.23	BTKB
ATOM	2652	O	PRO	469	36.312	39.718	30.592	1.00	34.40	BTKB
ATOM	2653	N	ILE	470	34.279	38.884	31.101	1.00	33.52	BTKB
ATOM	2654	CA	ILE	470	34.393	39.182	32.523	1.00	33.35	BTKB
ATOM	2655	CB	ILE	470	33.078	38.936	33.271	1.00	31.28	BTKB
ATOM	2656	CG2	ILE	470	33.265	39.263	34.737	1.00	32.57	BTKB
ATOM	2657	CG1	ILE	470	31.945	39.779	32.669	1.00	31.65	BTKB
ATOM	2658	CD	ILE	470	32.076	41.265	32.915	1.00	29.56	BTKB
ATOM	2659	C	ILE	470	35.489	38.369	33.187	1.00	34.04	BTKB
ATOM	2660	O	ILE	470	35.424	37.145	33.247	1.00	36.53	BTKB
ATOM	2661	N	PHE	471	36.511	39.064	33.662	1.00	33.94	BTKB

	Atom Number	Atom Type	Amino Acid Residue		X	Y	Z	Occ.	Temp Factor	
ATOM	2662	CA	PHE	471	37.623	38.412	34.322	1.00	33.78	BTKB
ATOM	2663	CB	PHE	471	38.894	39.254	34.174	1.00	34.34	BTKB
ATOM	2664	CG	PHE	471	39.606	39.058	32.865	1.00	32.47	BTKB
ATOM	2665	CD1	PHE	471	39.345	37.942	32.072	1.00	35.03	BTKB
ATOM	2666	CD2	PHE	471	40.573	39.962	32.448	1.00	29.92	BTKB
ATOM	2667	CE1	PHE	471	40.039	37.728	30.893	1.00	31.59	BTKB
ATOM	2668	CE2	PHE	471	41.272	39.755	31.270	1.00	31.32	BTKB
ATOM	2669	CZ	PHE	471	41.005	38.632	30.491	1.00	30.64	BTKB
ATOM	2670	C	PHE	471	37.301	38.186	35.792	1.00	34.09	BTKB
ATOM	2671	O	PHE	471	37.641	39.016	36.648	1.00	34.23	BTKB
ATOM	2672	N	ILE	472	36.580	37.102	36.069	1.00	31.42	BTKB
ATOM	2673	CA	ILE	472	36.224	36.754	37.438	1.00	25.25	BTKB
ATOM	2674	CB	ILE	472	34.991	35.817	37.493	1.00	25.15	BTKB
ATOM	2675	CG2	ILE	472	34.630	35.487	38.947	1.00	19.45	BTKB
ATOM	2676	CG1	ILE	472	33.795	36.493	36.816	1.00	23.77	BTKB
ATOM	2677	CD	ILE	472	32.512	35.683	36.860	1.00	27.24	BTKB
ATOM	2678	C	ILE	472	37.442	36.058	38.021	1.00	24.31	BTKB
ATOM	2679	O	ILE	472	38.127	35.307	37.321	1.00	21.85	BTKB
ATOM	2680	N	ILE	473	37.734	36.346	39.284	1.00	24.30	BTKB
ATOM	2681	CA	ILE	473	38.885	35.767	39.965	1.00	22.53	BTKB
ATOM	2682	CB	ILE	473	39.907	36.880	40.353	1.00	19.77	BTKB
ATOM	2683	CG2	ILE	473	40.447	36.702	41.771	1.00	21.00	BTKB
ATOM	2684	CG1	ILE	473	41.050	36.916	39.337	1.00	19.04	BTKB
ATOM	2685	CD	ILE	473	40.677	37.512	38.014	1.00	11.67	BTKB
ATOM	2686	C	ILE	473	38.478	34.914	41.168	1.00	22.23	BTKB
ATOM	2687	O	ILE	473	37.846	35.401	42.112	1.00	18.66	BTKB
ATOM	2688	N	THR	474	38.840	33.635	41.116	1.00	22.87	BTKB
ATOM	2689	CA	THR	474	38.517	32.699	42.179	1.00	20.65	BTKB
ATOM	2690	CB	THR	474	37.578	31.586	41.668	1.00	21.70	BTKB
ATOM	2691	OG1	THR	474	38.161	30.959	40.521	1.00	16.76	BTKB
ATOM	2692	CG2	THR	474	36.211	32.158	41.296	1.00	19.49	BTKB
ATOM	2693	C	THR	474	39.749	32.055	42.811	1.00	19.89	BTKB
ATOM	2694	O	THR	474	40.882	32.284	42.379	1.00	19.24	BTKB
ATOM	2695	N	GLU	475	39.499	31.234	43.826	1.00	17.71	BTKB
ATOM	2696	CA	GLU	475	40.528	30.526	44.577	1.00	18.24	BTKB
ATOM	2697	CB	GLU	475	39.878	29.940	45.834	1.00	17.97	BTKB
ATOM	2698	CG	GLU	475	40.814	29.304	46.846	1.00	24.32	BTKB
ATOM	2699	CD	GLU	475	40.076	28.796	48.080	1.00	27.60	BTKB
ATOM	2700	OE1	GLU	475	40.701	28.726	49.160	1.00	28.93	BTKB
ATOM	2701	OE2	GLU	475	38.872	28.468	47.972	1.00	29.54	BTKB
ATOM	2702	C	GLU	475	41.199	29.425	43.742	1.00	19.31	BTKB
ATOM	2703	O	GLU	475	40.538	28.495	43.271	1.00	21.47	BTKB
ATOM	2704	N	TYR	476	42.508	29.548	43.537	1.00	18.96	BTKB
ATOM	2705	CA	TYR	476	43.253	28.559	42.760	1.00	19.32	BTKB
ATOM	2706	CB	TYR	476	44.673	29.054	42.436	1.00	18.59	BTKB
ATOM	2707	CG	TYR	476	45.437	28.101	41.545	1.00	16.62	BTKB
ATOM	2708	CD1	TYR	476	45.097	27.963	40.204	1.00	16.76	BTKB
ATOM	2709	CE1	TYR	476	45.703	27.000	39.396	1.00	17.33	BTKB
ATOM	2710	CD2	TYR	476	46.419	27.259	42.064	1.00	18.86	BTKB
ATOM	2711	CE2	TYR	476	47.031	26.286	41.262	1.00	20.19	BTKB
ATOM	2712	CZ	TYR	476	46.660	26.164	39.929	1.00	18.14	BTKB
ATOM	2713	OH	TYR	476	47.206	25.182	39.134	1.00	15.15	BTKB
ATOM	2714	C	TYR	476	43.329	27.242	43.524	1.00	20.78	BTKB
ATOM	2715	O	TYR	476	43.758	27.208	44.678	1.00	21.62	BTKB
ATOM	2716	N	MET	477	42.925	26.158	42.871	1.00	17.28	BTKB
ATOM	2717	CA	MET	477	42.947	24.844	43.499	1.00	13.93	BTKB
ATOM	2718	CB	MET	477	41.552	24.232	43.458	1.00	10.54	BTKB
ATOM	2719	CG	MET	477	40.506	25.096	44.152	1.00	13.09	BTKB

	Atom Number	Atom Type	Amino Acid Residue		X	Y	Z	Occ.	Temp Factor	
ATOM	2720	SD	MET	477	40.797	25.261	45.909	1.00	14.13	BTKB
ATOM	2721	CE	MET	477	39.882	23.854	46.522	1.00	10.24	BTKB
ATOM	2722	C	MET	477	43.960	23.955	42.812	1.00	11.92	BTKB
ATOM	2723	O	MET	477	43.679	23.356	41.787	1.00	15.97	BTKB
ATOM	2724	N	ALA	478	45.131	23.851	43.425	1.00	12.80	BTKB
ATOM	2725	CA	ALA	478	46.260	23.087	42.908	1.00	11.29	BTKB
ATOM	2726	CB	ALA	478	47.397	23.091	43.927	1.00	10.32	BTKB
ATOM	2727	C	ALA	478	46.042	21.673	42.382	1.00	12.60	BTKB
ATOM	2728	O	ALA	478	46.767	21.239	41.479	1.00	11.34	BTKB
ATOM	2729	N	ASN	479	45.075	20.946	42.934	1.00	12.61	BTKB
ATOM	2730	CA	ASN	479	44.852	19.578	42.477	1.00	15.20	BTKB
ATOM	2731	CB	ASN	479	44.737	18.616	43.658	1.00	13.56	BTKB
ATOM	2732	CG	ASN	479	46.096	18.176	44.181	1.00	11.21	BTKB
ATOM	2733	OD1	ASN	479	46.963	17.763	43.418	1.00	11.71	BTKB
ATOM	2734	ND2	ASN	479	46.284	18.265	45.484	1.00	13.16	BTKB
ATOM	2735	C	ASN	479	43.714	19.367	41.494	1.00	14.96	BTKB
ATOM	2736	O	ASN	479	43.370	18.230	41.181	1.00	16.66	BTKB
ATOM	2737	N	GLY	480	43.160	20.467	40.985	1.00	16.33	BTKB
ATOM	2738	CA	GLY	480	42.080	20.406	40.011	1.00	16.11	BTKB
ATOM	2739	C	GLY	480	40.744	19.930	40.535	1.00	15.18	BTKB
ATOM	2740	O	GLY	480	40.427	20.112	41.705	1.00	16.02	BTKB
ATOM	2741	N	CYS	481	39.954	19.318	39.660	1.00	15.40	BTKB
ATOM	2742	CA	CYS	481	38.631	18.818	40.032	1.00	16.10	BTKB
ATOM	2743	CB	CYS	481	37.726	18.767	38.804	1.00	17.50	BTKB
ATOM	2744	SG	CYS	481	38.151	17.459	37.637	1.00	26.46	BTKB
ATOM	2745	C	CYS	481	38.663	17.440	40.706	1.00	13.33	BTKB
ATOM	2746	O	CYS	481	39.484	16.586	40.359	1.00	9.78	BTKB
ATOM	2747	N	LEU	482	37.716	17.218	41.620	1.00	12.03	BTKB
ATOM	2748	CA	LEU	482	37.581	15.966	42.367	1.00	12.13	BTKB
ATOM	2749	CB	LEU	482	36.390	16.058	43.340	1.00	12.80	BTKB
ATOM	2750	CG	LEU	482	36.066	14.923	44.327	1.00	10.31	BTKB
ATOM	2751	CD1	LEU	482	37.227	14.696	45.280	1.00	12.16	BTKB
ATOM	2752	CD2	LEU	482	34.792	15.233	45.114	1.00	12.14	BTKB
ATOM	2753	C	LEU	482	37.439	14.740	41.461	1.00	10.56	BTKB
ATOM	2754	O	LEU	482	38.066	13.714	41.714	1.00	11.00	BTKB
ATOM	2755	N	LEU	483	36.649	14.849	40.394	1.00	10.48	BTKB
ATOM	2756	CA	LEU	483	36.451	13.733	39.456	1.00	9.01	BTKB
ATOM	2757	CB	LEU	483	35.600	14.167	38.261	1.00	4.67	BTKB
ATOM	2758	CG	LEU	483	34.174	13.645	38.133	1.00	6.66	BTKB
ATOM	2759	CD1	LEU	483	33.737	13.825	36.691	1.00	7.76	BTKB
ATOM	2760	CD2	LEU	483	34.097	12.179	38.517	1.00	6.83	BTKB
ATOM	2761	C	LEU	483	37.763	13.170	38.925	1.00	13.13	BTKB
ATOM	2762	O	LEU	483	37.927	11.957	38.815	1.00	15.11	BTKB
ATOM	2763	N	ASN	484	38.679	14.064	38.562	1.00	15.95	BTKB
ATOM	2764	CA	ASN	484	39.990	13.673	38.047	1.00	18.08	BTKB
ATOM	2765	CB	ASN	484	40.689	14.855	37.371	1.00	22.13	BTKB
ATOM	2766	CG	ASN	484	39.864	15.473	36.265	1.00	23.79	BTKB
ATOM	2767	OD1	ASN	484	40.012	16.657	35.964	1.00	28.81	BTKB
ATOM	2768	ND2	ASN	484	38.991	14.682	35.651	1.00	29.42	BTKB
ATOM	2769	C	ASN	484	40.867	13.194	39.184	1.00	16.80	BTKB
ATOM	2770	O	ASN	484	41.790	12.415	38.977	1.00	16.25	BTKB
ATOM	2771	N	TYR	485	40.597	13.696	40.382	1.00	16.90	BTKB
ATOM	2772	CA	TYR	485	41.368	13.317	41.552	1.00	15.39	BTKB
ATOM	2773	CB	TYR	485	41.053	14.260	42.713	1.00	15.38	BTKB
ATOM	2774	CG	TYR	485	42.182	14.400	43.692	1.00	10.91	BTKB
ATOM	2775	CD1	TYR	485	43.446	14.782	43.263	1.00	10.29	BTKB
ATOM	2776	CE1	TYR	485	44.496	14.935	44.160	1.00	9.78	BTKB
ATOM	2777	CD2	TYR	485	41.989	14.166	45.050	1.00	13.87	BTKB

	Atom Number	Atom Type	Amino Acid Residue		X	Y	Z	Occ.	Temp Factor	
ATOM	2778	CE2	TYR	485	43.032	14.316	45.957	1.00	13.73	BTKB
ATOM	2779	CZ	TYR	485	44.284	14.704	45.501	1.00	14.21	BTKB
ATOM	2780	OH	TYR	485	45.322	14.890	46.389	1.00	20.03	BTKB
ATOM	2781	C	TYR	485	41.059	11.881	41.943	1.00	16.45	BTKB
ATOM	2782	O	TYR	485	41.957	11.066	42.096	1.00	20.72	BTKB
ATOM	2783	N	LEU	486	39.779	11.566	42.067	1.00	16.22	BTKB
ATOM	2784	CA	LEU	486	39.349	10.228	42.445	1.00	14.56	BTKB
ATOM	2785	CB	LEU	486	37.821	10.172	42.439	1.00	8.92	BTKB
ATOM	2786	CG	LEU	486	37.188	10.923	43.611	1.00	9.93	BTKB
ATOM	2787	CD1	LEU	486	35.698	11.154	43.365	1.00	6.93	BTKB
ATOM	2788	CD2	LEU	486	37.444	10.155	44.911	1.00	2.28	BTKB
ATOM	2789	C	LEU	486	39.935	9.123	41.561	1.00	17.58	BTKB
ATOM	2790	O	LEU	486	40.287	8.037	42.042	1.00	17.82	BTKB
ATOM	2791	N	ARG	487	40.054	9.413	40.272	1.00	22.23	BTKB
ATOM	2792	CA	ARG	487	40.589	8.457	39.313	1.00	24.99	BTKB
ATOM	2793	CB	ARG	487	40.060	8.786	37.914	1.00	25.06	BTKB
ATOM	2794	CG	ARG	487	38.543	8.776	37.775	1.00	25.61	BTKB
ATOM	2795	CD	ARG	487	37.994	7.357	37.693	1.00	34.03	BTKB
ATOM	2796	NE	ARG	487	37.266	7.113	36.445	1.00	36.39	BTKB
ATOM	2797	CZ	ARG	487	36.565	6.009	36.184	1.00	33.29	BTKB
ATOM	2798	NH1	ARG	487	36.492	5.034	37.083	1.00	31.06	BTKB
ATOM	2799	NH2	ARG	487	35.926	5.886	35.026	1.00	32.25	BTKB
ATOM	2800	C	ARG	487	42.117	8.481	39.297	1.00	25.69	BTKB
ATOM	2801	O	ARG	487	42.738	7.695	38.582	1.00	27.68	BTKB
ATOM	2802	N	GLU	488	42.713	9.341	40.121	1.00	29.95	BTKB
ATOM	2803	CA	GLU	488	44.164	9.507	40.168	1.00	32.26	BTKB
ATOM	2804	CB	GLU	488	44.618	10.299	41.405	1.00	35.45	BTKB
ATOM	2805	CG	GLU	488	44.416	9.609	42.751	1.00	35.63	BTKB
ATOM	2806	CD	GLU	488	45.086	10.359	43.902	1.00	36.03	BTKB
ATOM	2807	OE1	GLU	488	45.854	9.725	44.657	1.00	34.00	BTKB
ATOM	2808	OE2	GLU	488	44.857	11.578	44.050	1.00	30.65	BTKB
ATOM	2809	C	GLU	488	44.967	8.234	40.046	1.00	35.02	BTKB
ATOM	2810	O	GLU	488	44.680	7.234	40.704	1.00	36.27	BTKB
ATOM	2811	N	MET	489	45.975	8.304	39.178	1.00	39.21	BTKB
ATOM	2812	CA	MET	489	46.892	7.209	38.881	1.00	40.20	BTKB
ATOM	2813	CB	MET	489	48.243	7.779	38.437	1.00	40.38	BTKB
ATOM	2814	CG	MET	489	48.173	9.022	37.536	1.00	41.55	BTKB
ATOM	2815	SD	MET	489	47.548	8.779	35.843	1.00	43.59	BTKB
ATOM	2816	CE	MET	489	46.615	10.283	35.628	1.00	40.20	BTKB
ATOM	2817	C	MET	489	47.087	6.305	40.101	1.00	40.72	BTKB
ATOM	2818	O	MET	489	46.473	5.239	40.204	1.00	42.05	BTKB
ATOM	2819	N	ARG	490	47.930	6.744	41.028	1.00	40.79	BTKB
ATOM	2820	CA	ARG	490	48.195	5.995	42.245	1.00	37.42	BTKB
ATOM	2821	CB	ARG	490	49.437	6.553	42.932	1.00	33.39	BTKB
ATOM	2822	CG	ARG	490	50.727	6.263	42.195	1.00	33.75	BTKB
ATOM	2823	CD	ARG	490	51.220	4.849	42.479	1.00	29.04	BTKB
ATOM	2824	NE	ARG	490	52.596	4.854	42.970	1.00	27.07	BTKB
ATOM	2825	CZ	ARG	490	52.969	5.326	44.159	1.00	25.71	BTKB
ATOM	2826	NH1	ARG	490	52.067	5.827	44.996	1.00	21.84	BTKB
ATOM	2827	NH2	ARG	490	54.255	5.355	44.487	1.00	21.92	BTKB
ATOM	2828	C	ARG	490	46.983	6.127	43.156	1.00	37.49	BTKB
ATOM	2829	O	ARG	490	46.884	7.076	43.933	1.00	33.88	BTKB
ATOM	2830	N	HIS	491	46.063	5.172	43.047	1.00	37.72	BTKB
ATOM	2831	CA	HIS	491	44.826	5.166	43.833	1.00	35.57	BTKB
ATOM	2832	CB	HIS	491	43.863	4.096	43.288	1.00	34.70	BTKB
ATOM	2833	CG	HIS	491	43.450	4.303	41.859	1.00	34.85	BTKB
ATOM	2834	CD2	HIS	491	42.253	4.634	41.321	1.00	33.61	BTKB
ATOM	2835	ND1	HIS	491	44.312	4.133	40.797	1.00	34.49	BTKB

	Atom Number	Atom Type	Amino Acid Residue		X	Y	Z	Occ.	Temp Factor	
ATOM	2836	CE1	HIS	491	43.664	4.348	39.665	1.00	32.88	BTKB
ATOM	2837	NE2	HIS	491	42.413	4.654	39.956	1.00	33.96	BTKB
ATOM	2838	C	HIS	491	45.068	4.915	45.327	1.00	33.29	BTKB
ATOM	2839	O	HIS	491	44.479	4.007	45.913	1.00	34.31	BTKB
ATOM	2840	N	ARG	492	45.921	5.723	45.948	1.00	31.88	BTKB
ATOM	2841	CA	ARG	492	46.228	5.561	47.362	1.00	31.93	BTKB
ATOM	2842	CB	ARG	492	47.566	6.224	47.697	1.00	32.51	BTKB
ATOM	2843	CG	ARG	492	48.746	5.765	46.847	1.00	35.36	BTKB
ATOM	2844	CD	ARG	492	50.013	6.544	47.196	1.00	33.65	BTKB
ATOM	2845	NE	ARG	492	49.859	7.979	46.958	1.00	33.39	BTKB
ATOM	2846	CZ	ARG	492	50.807	8.886	47.169	1.00	29.63	BTKB
ATOM	2847	NH1	ARG	492	51.994	8.525	47.626	1.00	22.52	BTKB
ATOM	2848	NH2	ARG	492	50.559	10.163	46.941	1.00	28.36	BTKB
ATOM	2849	C	ARG	492	45.123	6.221	48.165	1.00	33.93	BTKB
ATOM	2850	O	ARG	492	45.323	7.295	48.730	1.00	36.87	BTKB
ATOM	2851	N	PHE	493	43.953	5.591	48.201	1.00	32.16	BTKB
ATOM	2852	CA	PHE	493	42.824	6.148	48.932	1.00	30.58	BTKB
ATOM	2853	CB	PHE	493	41.708	6.587	47.974	1.00	28.91	BTKB
ATOM	2854	CG	PHE	493	41.862	7.993	47.466	1.00	22.07	BTKB
ATOM	2855	CD1	PHE	493	42.001	8.247	46.110	1.00	23.04	BTKB
ATOM	2856	CD2	PHE	493	41.880	9.062	48.352	1.00	20.91	BTKB
ATOM	2857	CE1	PHE	493	42.159	9.549	45.642	1.00	21.21	BTKB
ATOM	2858	CE2	PHE	493	42.037	10.361	47.898	1.00	18.07	BTKB
ATOM	2859	CZ	PHE	493	42.178	10.606	46.536	1.00	23.31	BTKB
ATOM	2860	C	PHE	493	42.256	5.207	49.976	1.00	30.49	BTKB
ATOM	2861	O	PHE	493	41.858	4.079	49.676	1.00	30.95	BTKB
ATOM	2862	N	GLN	494	42.240	5.679	51.213	1.00	29.40	BTKB
ATOM	2863	CA	GLN	494	41.702	4.907	52.320	1.00	28.93	BTKB
ATOM	2864	CB	GLN	494	42.640	4.985	53.529	1.00	31.31	BTKB
ATOM	2865	CG	GLN	494	44.047	4.427	53.298	1.00	35.24	BTKB
ATOM	2866	CD	GLN	494	45.041	5.495	52.888	1.00	36.73	BTKB
ATOM	2867	OE1	GLN	494	44.778	6.289	51.984	1.00	36.12	BTKB
ATOM	2868	NE2	GLN	494	46.184	5.529	53.559	1.00	34.99	BTKB
ATOM	2869	C	GLN	494	40.337	5.499	52.660	1.00	26.79	BTKB
ATOM	2870	O	GLN	494	40.132	6.707	52.516	1.00	30.22	BTKB
ATOM	2871	N	THR	495	39.405	4.660	53.104	1.00	24.49	BTKB
ATOM	2872	CA	THR	495	38.059	5.107	53.453	1.00	18.71	BTKB
ATOM	2873	CB	THR	495	37.261	3.983	54.136	1.00	15.78	BTKB
ATOM	2874	OG1	THR	495	37.282	2.823	53.302	1.00	17.79	BTKB
ATOM	2875	CG2	THR	495	35.814	4.405	54.359	1.00	12.00	BTKB
ATOM	2876	C	THR	495	38.083	6.320	54.372	1.00	19.04	BTKB
ATOM	2877	O	THR	495	37.209	7.182	54.299	1.00	19.97	BTKB
ATOM	2878	N	GLN	496	39.112	6.393	55.207	1.00	20.71	BTKB
ATOM	2879	CA	GLN	496	39.285	7.488	56.156	1.00	20.37	BTKB
ATOM	2880	CB	GLN	496	40.605	7.320	56.930	1.00	24.38	BTKB
ATOM	2881	CG	GLN	496	40.686	6.083	57.852	1.00	31.81	BTKB
ATOM	2882	CD	GLN	496	40.842	4.747	57.107	1.00	35.85	BTKB
ATOM	2883	OE1	GLN	496	41.121	4.714	55.909	1.00	33.78	BTKB
ATOM	2884	NE2	GLN	496	40.660	3.643	57.825	1.00	34.70	BTKB
ATOM	2885	C	GLN	496	39.282	8.825	55.419	1.00	18.15	BTKB
ATOM	2886	O	GLN	496	38.519	9.725	55.748	1.00	18.72	BTKB
ATOM	2887	N	GLN	497	40.114	8.935	54.393	1.00	18.73	BTKB
ATOM	2888	CA	GLN	497	40.205	10.162	53.615	1.00	14.92	BTKB
ATOM	2889	CB	GLN	497	41.534	10.196	52.862	1.00	21.68	BTKB
ATOM	2890	CG	GLN	497	41.752	11.477	52.090	1.00	25.81	BTKB
ATOM	2891	CD	GLN	497	41.416	12.694	52.912	1.00	25.45	BTKB
ATOM	2892	OE1	GLN	497	41.984	12.911	53.985	1.00	30.13	BTKB
ATOM	2893	NE2	GLN	497	40.462	13.480	52.434	1.00	22.53	BTKB

	Atom Number	Atom Type	Amino Acid Residue		X	Y	Z	Occ.	Temp Factor	
ATOM	2894	C	GLN	497	39.031	10.315	52.647	1.00	11.54	BTKB
ATOM	2895	O	GLN	497	38.656	11.425	52.272	1.00	10.10	BTKB
ATOM	2896	N	LEU	498	38.463	9.189	52.240	1.00	9.12	BTKB
ATOM	2897	CA	LEU	498	37.327	9.173	51.336	1.00	8.57	BTKB
ATOM	2898	CB	LEU	498	36.961	7.721	51.021	1.00	11.37	BTKB
ATOM	2899	CG	LEU	498	36.951	7.223	49.575	1.00	9.98	BTKB
ATOM	2900	CD1	LEU	498	38.079	7.838	48.767	1.00	8.19	BTKB
ATOM	2901	CD2	LEU	498	37.050	5.711	49.570	1.00	7.91	BTKB
ATOM	2902	C	LEU	498	36.167	9.868	52.043	1.00	10.48	BTKB
ATOM	2903	O	LEU	498	35.469	10.702	51.458	1.00	11.51	BTKB
ATOM	2904	N	LEU	499	36.016	9.569	53.331	1.00	12.46	BTKB
ATOM	2905	CA	LEU	499	34.949	10.146	54.133	1.00	10.83	BTKB
ATOM	2906	CB	LEU	499	34.815	9.375	55.454	1.00	12.04	BTKB
ATOM	2907	CG	LEU	499	33.474	9.303	56.205	1.00	8.53	BTKB
ATOM	2908	CD1	LEU	499	33.416	10.349	57.280	1.00	8.11	BTKB
ATOM	2909	CD2	LEU	499	32.286	9.415	55.263	1.00	5.87	BTKB
ATOM	2910	C	LEU	499	35.229	11.622	54.365	1.00	7.37	BTKB
ATOM	2911	O	LEU	499	34.327	12.449	54.275	1.00	10.84	BTKB
ATOM	2912	N	GLU	500	36.491	11.960	54.607	1.00	8.33	BTKB
ATOM	2913	CA	GLU	500	36.878	13.353	54.821	1.00	10.19	BTKB
ATOM	2914	CB	GLU	500	38.407	13.498	54.933	1.00	11.71	BTKB
ATOM	2915	CG	GLU	500	38.988	13.251	56.326	1.00	15.65	BTKB
ATOM	2916	CD	GLU	500	38.574	14.307	57.342	1.00	16.85	BTKB
ATOM	2917	OE1	GLU	500	38.534	13.992	58.550	1.00	17.26	BTKB
ATOM	2918	OE2	GLU	500	38.290	15.454	56.940	1.00	21.13	BTKB
ATOM	2919	C	GLU	500	36.377	14.220	53.679	1.00	10.00	BTKB
ATOM	2920	O	GLU	500	35.914	15.328	53.898	1.00	12.10	BTKB
ATOM	2921	N	MET	501	36.453	13.701	52.459	1.00	12.06	BTKB
ATOM	2922	CA	MET	501	36.009	14.434	51.284	1.00	11.31	BTKB
ATOM	2923	CB	MET	501	36.314	13.637	50.015	1.00	10.59	BTKB
ATOM	2924	CG	MET	501	37.792	13.351	49.803	1.00	11.63	BTKB
ATOM	2925	SD	MET	501	38.095	12.353	48.335	1.00	16.64	BTKB
ATOM	2926	CE	MET	501	39.512	13.180	47.631	1.00	19.96	BTKB
ATOM	2927	C	MET	501	34.522	14.720	51.400	1.00	11.74	BTKB
ATOM	2928	O	MET	501	34.098	15.865	51.257	1.00	12.06	BTKB
ATOM	2929	N	CYS	502	33.740	13.685	51.707	1.00	11.26	BTKB
ATOM	2930	CA	CYS	502	32.290	13.818	51.879	1.00	10.20	BTKB
ATOM	2931	CB	CYS	502	31.673	12.473	52.290	1.00	12.20	BTKB
ATOM	2932	SG	CYS	502	31.964	11.065	51.174	1.00	14.20	BTKB
ATOM	2933	C	CYS	502	31.986	14.848	52.976	1.00	9.69	BTKB
ATOM	2934	O	CYS	502	30.976	15.549	52.923	1.00	7.12	BTKB
ATOM	2935	N	LYS	503	32.872	14.924	53.967	1.00	11.41	BTKB
ATOM	2936	CA	LYS	503	32.735	15.838	55.095	1.00	7.79	BTKB
ATOM	2937	CB	LYS	503	33.700	15.431	56.217	1.00	4.87	BTKB
ATOM	2938	CG	LYS	503	33.559	16.217	57.519	1.00	7.28	BTKB
ATOM	2939	CD	LYS	503	34.929	16.669	58.024	1.00	12.59	BTKB
ATOM	2940	CE	LYS	503	34.879	17.121	59.483	1.00	12.64	BTKB
ATOM	2941	NZ	LYS	503	36.120	17.842	59.917	1.00	16.35	BTKB
ATOM	2942	C	LYS	503	32.993	17.280	54.656	1.00	7.32	BTKB
ATOM	2943	O	LYS	503	32.235	18.185	54.997	1.00	9.67	BTKB
ATOM	2944	N	ASP	504	34.051	17.484	53.883	1.00	4.47	BTKB
ATOM	2945	CA	ASP	504	34.401	18.801	53.387	1.00	2.00	BTKB
ATOM	2946	CB	ASP	504	35.649	18.712	52.505	1.00	5.96	BTKB
ATOM	2947	CG	ASP	504	36.876	18.212	53.253	1.00	5.96	BTKB
ATOM	2948	OD1	ASP	504	36.861	18.172	54.500	1.00	6.58	BTKB
ATOM	2949	OD2	ASP	504	37.863	17.856	52.580	1.00	11.77	BTKB
ATOM	2950	C	ASP	504	33.244	19.350	52.566	1.00	6.17	BTKB
ATOM	2951	O	ASP	504	32.857	20.512	52.723	1.00	4.62	BTKB

	Atom Number	Atom Type	Amino Acid Residue		X	Y	Z	Occ.	Temp Factor	
ATOM	2952	N	VAL	505	32.680	18.499	51.705	1.00	8.12	BTKB
ATOM	2953	CA	VAL	505	31.560	18.880	50.841	1.00	5.94	BTKB
ATOM	2954	CB	VAL	505	31.241	17.800	49.763	1.00	2.00	BTKB
ATOM	2955	CG1	VAL	505	30.116	18.283	48.867	1.00	3.28	BTKB
ATOM	2956	CG2	VAL	505	32.466	17.495	48.918	1.00	5.68	BTKB
ATOM	2957	C	VAL	505	30.294	19.109	51.652	1.00	7.08	BTKB
ATOM	2958	O	VAL	505	29.560	20.069	51.415	1.00	9.90	BTKB
ATOM	2959	N	CYS	506	30.050	18.235	52.622	1.00	8.09	BTKB
ATOM	2960	CA	CYS	506	28.861	18.336	53.444	1.00	8.75	BTKB
ATOM	2961	CB	CYS	506	28.728	17.112	54.355	1.00	7.47	BTKB
ATOM	2962	SG	CYS	506	27.033	16.791	54.882	1.00	8.97	BTKB
ATOM	2963	C	CYS	506	28.856	19.621	54.257	1.00	8.23	BTKB
ATOM	2964	O	CYS	506	27.822	20.272	54.378	1.00	10.16	BTKB
ATOM	2965	N	GLU	507	30.010	20.000	54.796	1.00	8.06	BTKB
ATOM	2966	CA	GLU	507	30.112	21.226	55.588	1.00	8.72	BTKB
ATOM	2967	CB	GLU	507	31.532	21.409	56.118	1.00	5.94	BTKB
ATOM	2968	CG	GLU	507	31.986	20.276	57.018	1.00	8.44	BTKB
ATOM	2969	CD	GLU	507	33.360	20.479	57.612	1.00	5.09	BTKB
ATOM	2970	OE1	GLU	507	34.090	21.392	57.197	1.00	12.55	BTKB
ATOM	2971	OE2	GLU	507	33.714	19.708	58.514	1.00	12.74	BTKB
ATOM	2972	C	GLU	507	29.727	22.422	54.730	1.00	9.87	BTKB
ATOM	2973	O	GLU	507	28.948	23.286	55.152	1.00	14.35	BTKB
ATOM	2974	N	ALA	508	30.272	22.460	53.518	1.00	10.59	BTKB
ATOM	2975	CA	ALA	508	30.001	23.530	52.568	1.00	10.69	BTKB
ATOM	2976	CB	ALA	508	30.859	23.337	51.343	1.00	11.50	BTKB
ATOM	2977	C	ALA	508	28.521	23.542	52.183	1.00	10.30	BTKB
ATOM	2978	O	ALA	508	27.885	24.597	52.110	1.00	7.78	BTKB
ATOM	2979	N	MET	509	27.983	22.355	51.929	1.00	11.26	BTKB
ATOM	2980	CA	MET	509	26.582	22.212	51.556	1.00	13.26	BTKB
ATOM	2981	CB	MET	509	26.301	20.796	51.053	1.00	12.49	BTKB
ATOM	2982	CG	MET	509	26.833	20.504	49.671	1.00	9.20	BTKB
ATOM	2983	SD	MET	509	26.595	21.913	48.607	1.00	9.16	BTKB
ATOM	2984	CE	MET	509	24.812	21.976	48.456	1.00	5.81	BTKB
ATOM	2985	C	MET	509	25.679	22.514	52.738	1.00	17.44	BTKB
ATOM	2986	O	MET	509	24.539	22.961	52.570	1.00	19.95	BTKB
ATOM	2987	N	GLU	510	26.198	22.251	53.932	1.00	18.37	BTKB
ATOM	2988	CA	GLU	510	25.467	22.479	55.159	1.00	17.75	BTKB
ATOM	2989	CB	GLU	510	26.217	21.858	56.336	1.00	21.22	BTKB
ATOM	2990	CG	GLU	510	25.370	21.629	57.572	1.00	19.10	BTKB
ATOM	2991	CD	GLU	510	25.692	22.587	58.687	1.00	21.96	BTKB
ATOM	2992	OE1	GLU	510	26.774	22.452	59.296	1.00	20.26	BTKB
ATOM	2993	OE2	GLU	510	24.859	23.472	58.958	1.00	24.99	BTKB
ATOM	2994	C	GLU	510	25.293	23.981	55.335	1.00	19.15	BTKB
ATOM	2995	O	GLU	510	24.178	24.446	55.579	1.00	21.52	BTKB
ATOM	2996	N	TYR	511	26.368	24.751	55.169	1.00	19.18	BTKB
ATOM	2997	CA	TYR	511	26.251	26.204	55.299	1.00	22.64	BTKB
ATOM	2998	CB	TYR	511	27.612	26.885	55.456	1.00	28.60	BTKB
ATOM	2999	CG	TYR	511	27.764	27.549	56.815	1.00	38.15	BTKB
ATOM	3000	CD1	TYR	511	27.179	26.988	57.958	1.00	38.05	BTKB
ATOM	3001	CE1	TYR	511	27.291	27.597	59.199	1.00	39.84	BTKB
ATOM	3002	CD2	TYR	511	28.469	28.745	56.958	1.00	37.94	BTKB
ATOM	3003	CE2	TYR	511	28.589	29.365	58.206	1.00	38.73	BTKB
ATOM	3004	CZ	TYR	511	27.995	28.786	59.319	1.00	40.24	BTKB
ATOM	3005	OH	TYR	511	28.100	29.397	60.550	1.00	37.79	BTKB
ATOM	3006	C	TYR	511	25.441	26.838	54.168	1.00	20.77	BTKB
ATOM	3007	O	TYR	511	24.824	27.881	54.353	1.00	19.57	BTKB
ATOM	3008	N	LEU	512	25.460	26.223	52.991	1.00	21.25	BTKB
ATOM	3009	CA	LEU	512	24.662	26.734	51.885	1.00	18.82	BTKB

	Atom Number	Atom Type	Amino Acid Residue		X	Y	Z	Occ.	Temp Factor	
ATOM	3010	CB	LEU	512	24.985	26.022	50.569	1.00	17.08	BTKB
ATOM	3011	CG	LEU	512	26.256	26.418	49.811	1.00	16.90	BTKB
ATOM	3012	CD1	LEU	512	26.165	25.864	48.375	1.00	10.52	BTKB
ATOM	3013	CD2	LEU	512	26.414	27.937	49.783	1.00	10.86	BTKB
ATOM	3014	C	LEU	512	23.217	26.473	52.271	1.00	19.11	BTKB
ATOM	3015	O	LEU	512	22.354	27.328	52.097	1.00	23.50	BTKB
ATOM	3016	N	GLU	513	22.972	25.306	52.851	1.00	19.26	BTKB
ATOM	3017	CA	GLU	513	21.640	24.930	53.283	1.00	18.74	BTKB
ATOM	3018	CB	GLU	513	21.665	23.554	53.944	1.00	16.46	BTKB
ATOM	3019	CG	GLU	513	20.296	23.079	54.393	1.00	18.68	BTKB
ATOM	3020	CD	GLU	513	20.327	21.695	55.003	1.00	17.60	BTKB
ATOM	3021	OE1	GLU	513	19.879	20.746	54.322	1.00	17.80	BTKB
ATOM	3022	OE2	GLU	513	20.792	21.561	56.159	1.00	12.10	BTKB
ATOM	3023	C	GLU	513	21.123	25.962	54.269	1.00	22.83	BTKB
ATOM	3024	O	GLU	513	20.033	26.514	54.079	1.00	26.96	BTKB
ATOM	3025	N	SER	514	21.924	26.241	55.300	1.00	24.79	BTKB
ATOM	3026	CA	SER	514	21.573	27.212	56.338	1.00	24.05	BTKB
ATOM	3027	CB	SER	514	22.693	27.314	57.376	1.00	23.79	BTKB
ATOM	3028	OG	SER	514	23.886	27.829	56.799	1.00	22.03	BTKB
ATOM	3029	C	SER	514	21.325	28.589	55.733	1.00	22.16	BTKB
ATOM	3030	O	SER	514	20.357	29.263	56.080	1.00	21.49	BTKB
ATOM	3031	N	LYS	515	22.195	28.974	54.805	1.00	21.78	BTKB
ATOM	3032	CA	LYS	515	22.128	30.263	54.122	1.00	19.84	BTKB
ATOM	3033	CB	LYS	515	23.522	30.574	53.541	1.00	15.28	BTKB
ATOM	3034	CG	LYS	515	23.593	31.460	52.308	1.00	22.32	BTKB
ATOM	3035	CD	LYS	515	23.373	32.930	52.616	1.00	20.90	BTKB
ATOM	3036	CE	LYS	515	23.192	33.703	51.322	1.00	15.11	BTKB
ATOM	3037	NZ	LYS	515	22.035	33.175	50.535	1.00	9.55	BTKB
ATOM	3038	C	LYS	515	21.008	30.302	53.072	1.00	20.47	BTKB
ATOM	3039	O	LYS	515	20.769	31.325	52.433	1.00	22.75	BTKB
ATOM	3040	N	GLN	516	20.267	29.206	52.956	1.00	19.94	BTKB
ATOM	3041	CA	GLN	516	19.165	29.111	52.000	1.00	19.73	BTKB
ATOM	3042	CB	GLN	516	18.085	30.162	52.314	1.00	23.43	BTKB
ATOM	3043	CG	GLN	516	17.672	30.281	53.783	1.00	22.95	BTKB
ATOM	3044	CD	GLN	516	16.919	29.073	54.296	1.00	30.24	BTKB
ATOM	3045	OE1	GLN	516	15.719	28.929	54.063	1.00	32.30	BTKB
ATOM	3046	NE2	GLN	516	17.612	28.212	55.026	1.00	32.64	BTKB
ATOM	3047	C	GLN	516	19.658	29.287	50.554	1.00	17.78	BTKB
ATOM	3048	O	GLN	516	19.000	29.935	49.733	1.00	15.79	BTKB
ATOM	3049	N	PHE	517	20.788	28.669	50.231	1.00	13.90	BTKB
ATOM	3050	CA	PHE	517	21.353	28.773	48.891	1.00	16.72	BTKB
ATOM	3051	CB	PHE	517	22.719	29.453	48.963	1.00	13.45	BTKB
ATOM	3052	CG	PHE	517	23.245	29.919	47.628	1.00	13.82	BTKB
ATOM	3053	CD1	PHE	517	23.067	31.246	47.220	1.00	11.73	BTKB
ATOM	3054	CD2	PHE	517	23.957	29.049	46.800	1.00	12.17	BTKB
ATOM	3055	CE1	PHE	517	23.596	31.699	46.002	1.00	11.02	BTKB
ATOM	3056	CE2	PHE	517	24.491	29.486	45.584	1.00	9.71	BTKB
ATOM	3057	CZ	PHE	517	24.312	30.815	45.183	1.00	13.73	BTKB
ATOM	3058	C	PHE	517	21.477	27.412	48.197	1.00	17.18	BTKB
ATOM	3059	O	PHE	517	22.222	26.540	48.658	1.00	20.28	BTKB
ATOM	3060	N	LEU	518	20.749	27.242	47.093	1.00	15.31	BTKB
ATOM	3061	CA	LEU	518	20.766	26.003	46.312	1.00	13.37	BTKB
ATOM	3062	CB	LEU	518	19.474	25.864	45.508	1.00	10.07	BTKB
ATOM	3063	CG	LEU	518	18.227	25.283	46.168	1.00	12.29	BTKB
ATOM	3064	CD1	LEU	518	17.018	25.488	45.274	1.00	9.13	BTKB
ATOM	3065	CD2	LEU	518	18.455	23.817	46.434	1.00	14.04	BTKB
ATOM	3066	C	LEU	518	21.936	25.979	45.334	1.00	13.97	BTKB
ATOM	3067	O	LEU	518	22.236	26.979	44.692	1.00	19.55	BTKB

	Atom Number	Atom Type	Amino Acid Residue		X	Y	Z	Occ.	Temp Factor	
ATOM	3068	N	HIS	519	22.557	24.820	45.165	1.00	13.91	BTKB
ATOM	3069	CA	HIS	519	23.684	24.700	44.250	1.00	15.81	BTKB
ATOM	3070	CB	HIS	519	24.659	23.631	44.743	1.00	12.29	BTKB
ATOM	3071	CG	HIS	519	26.008	23.706	44.101	1.00	9.16	BTKB
ATOM	3072	CD2	HIS	519	27.239	23.881	44.637	1.00	9.86	BTKB
ATOM	3073	ND1	HIS	519	26.198	23.578	42.741	1.00	7.69	BTKB
ATOM	3074	CE1	HIS	519	27.489	23.664	42.468	1.00	8.06	BTKB
ATOM	3075	NE2	HIS	519	28.142	23.850	43.602	1.00	9.01	BTKB
ATOM	3076	C	HIS	519	23.256	24.396	42.811	1.00	18.77	BTKB
ATOM	3077	O	HIS	519	23.987	24.714	41.877	1.00	19.63	BTKB
ATOM	3078	N	ARG	520	22.116	23.724	42.645	1.00	21.67	BTKB
ATOM	3079	CA	ARG	520	21.572	23.372	41.329	1.00	21.63	BTKB
ATOM	3080	CB	ARG	520	21.501	24.620	40.438	1.00	21.69	BTKB
ATOM	3081	CG	ARG	520	20.865	24.389	39.081	1.00	24.47	BTKB
ATOM	3082	CD	ARG	520	21.521	25.238	38.001	1.00	26.51	BTKB
ATOM	3083	NE	ARG	520	21.186	26.658	38.074	1.00	33.49	BTKB
ATOM	3084	CZ	ARG	520	20.034	27.185	37.667	1.00	32.52	BTKB
ATOM	3085	NH1	ARG	520	19.078	26.412	37.169	1.00	35.39	BTKB
ATOM	3086	NH2	ARG	520	19.870	28.502	37.675	1.00	36.18	BTKB
ATOM	3087	C	ARG	520	22.295	22.232	40.582	1.00	23.98	BTKB
ATOM	3088	O	ARG	520	21.646	21.366	39.987	1.00	23.54	BTKB
ATOM	3089	N	ASP	521	23.625	22.221	40.629	1.00	21.56	BTKB
ATOM	3090	CA	ASP	521	24.423	21.210	39.935	1.00	19.42	BTKB
ATOM	3091	CB	ASP	521	25.033	21.861	38.676	1.00	20.57	BTKB
ATOM	3092	CG	ASP	521	25.309	20.867	37.552	1.00	18.16	BTKB
ATOM	3093	OD1	ASP	521	26.470	20.777	37.099	1.00	19.83	BTKB
ATOM	3094	OD2	ASP	521	24.359	20.205	37.092	1.00	21.97	BTKB
ATOM	3095	C	ASP	521	25.533	20.709	40.872	1.00	17.08	BTKB
ATOM	3096	O	ASP	521	26.655	21.199	40.830	1.00	19.34	BTKB
ATOM	3097	N	LEU	522	25.206	19.781	41.763	1.00	14.72	BTKB
ATOM	3098	CA	LEU	522	26.197	19.252	42.704	1.00	12.04	BTKB
ATOM	3099	CB	LEU	522	25.612	19.164	44.117	1.00	15.80	BTKB
ATOM	3100	CG	LEU	522	26.527	18.661	45.235	1.00	15.39	BTKB
ATOM	3101	CD1	LEU	522	27.670	19.639	45.486	1.00	14.85	BTKB
ATOM	3102	CD2	LEU	522	25.709	18.455	46.490	1.00	14.89	BTKB
ATOM	3103	C	LEU	522	26.724	17.892	42.249	1.00	11.47	BTKB
ATOM	3104	O	LEU	522	25.991	16.902	42.200	1.00	8.58	BTKB
ATOM	3105	N	ALA	523	28.015	17.851	41.949	1.00	9.69	BTKB
ATOM	3106	CA	ALA	523	28.650	16.637	41.467	1.00	7.49	BTKB
ATOM	3107	CB	ALA	523	28.332	16.457	39.968	1.00	8.23	BTKB
ATOM	3108	C	ALA	523	30.150	16.780	41.677	1.00	3.64	BTKB
ATOM	3109	O	ALA	523	30.643	17.892	41.858	1.00	5.50	BTKB
ATOM	3110	N	ALA	524	30.880	15.671	41.609	1.00	2.00	BTKB
ATOM	3111	CA	ALA	524	32.328	15.695	41.804	1.00	3.96	BTKB
ATOM	3112	CB	ALA	524	32.890	14.289	41.820	1.00	2.49	BTKB
ATOM	3113	C	ALA	524	33.040	16.533	40.753	1.00	3.94	BTKB
ATOM	3114	O	ALA	524	34.159	16.994	40.974	1.00	2.00	BTKB
ATOM	3115	N	ARG	525	32.409	16.696	39.596	1.00	6.91	BTKB
ATOM	3116	CA	ARG	525	32.979	17.497	38.515	1.00	11.27	BTKB
ATOM	3117	CB	ARG	525	32.152	17.328	37.246	1.00	13.87	BTKB
ATOM	3118	CG	ARG	525	30.741	17.870	37.362	1.00	18.97	BTKB
ATOM	3119	CD	ARG	525	30.214	18.263	35.997	1.00	23.23	BTKB
ATOM	3120	NE	ARG	525	31.138	19.182	35.332	1.00	29.34	BTKB
ATOM	3121	CZ	ARG	525	30.855	20.439	35.010	1.00	30.92	BTKB
ATOM	3122	NH1	ARG	525	29.662	20.956	35.283	1.00	31.96	BTKB
ATOM	3123	NH2	ARG	525	31.773	21.183	34.412	1.00	28.24	BTKB
ATOM	3124	C	ARG	525	33.002	18.983	38.891	1.00	11.79	BTKB
ATOM	3125	O	ARG	525	33.802	19.760	38.376	1.00	11.27	BTKB

	Atom Number	Atom Type	Amino Acid Residue		X	Y	Z	Occ.	Temp Factor	
ATOM	3126	N	ASN	526	32.099	19.364	39.785	1.00	11.62	BTKB
ATOM	3127	CA	ASN	526	31.982	20.734	40.250	1.00	8.74	BTKB
ATOM	3128	CB	ASN	526	30.504	21.093	40.372	1.00	6.93	BTKB
ATOM	3129	CG	ASN	526	29.781	21.003	39.047	1.00	8.76	BTKB
ATOM	3130	OD1	ASN	526	28.796	20.275	38.909	1.00	13.72	BTKB
ATOM	3131	ND2	ASN	526	30.283	21.725	38.051	1.00	11.51	BTKB
ATOM	3132	C	ASN	526	32.698	20.956	41.585	1.00	5.24	BTKB
ATOM	3133	O	ASN	526	32.471	21.956	42.255	1.00	4.05	BTKB
ATOM	3134	N	CYS	527	33.549	20.013	41.977	1.00	7.78	BTKB
ATOM	3135	CA	CYS	527	34.302	20.128	43.218	1.00	9.39	BTKB
ATOM	3136	CB	CYS	527	34.046	18.934	44.147	1.00	8.89	BTKB
ATOM	3137	SG	CYS	527	32.439	18.919	44.970	1.00	9.13	BTKB
ATOM	3138	C	CYS	527	35.777	20.186	42.865	1.00	6.94	BTKB
ATOM	3139	O	CYS	527	36.225	19.505	41.942	1.00	9.40	BTKB
ATOM	3140	N	LEU	528	36.520	21.006	43.600	1.00	10.86	BTKB
ATOM	3141	CA	LEU	528	37.953	21.176	43.376	1.00	12.73	BTKB
ATOM	3142	CB	LEU	528	38.276	22.646	43.097	1.00	12.37	BTKB
ATOM	3143	CG	LEU	528	37.598	23.307	41.892	1.00	12.90	BTKB
ATOM	3144	CD1	LEU	528	37.402	24.781	42.185	1.00	19.16	BTKB
ATOM	3145	CD2	LEU	528	38.419	23.099	40.614	1.00	17.35	BTKB
ATOM	3146	C	LEU	528	38.734	20.710	44.591	1.00	12.40	BTKB
ATOM	3147	O	LEU	528	38.197	20.638	45.696	1.00	14.00	BTKB
ATOM	3148	N	VAL	529	40.009	20.405	44.381	1.00	13.66	BTKB
ATOM	3149	CA	VAL	529	40.884	19.939	45.446	1.00	16.38	BTKB
ATOM	3150	CB	VAL	529	41.324	18.477	45.205	1.00	13.16	BTKB
ATOM	3151	CG1	VAL	529	42.156	17.971	46.387	1.00	7.91	BTKB
ATOM	3152	CG2	VAL	529	40.105	17.586	44.943	1.00	15.41	BTKB
ATOM	3153	C	VAL	529	42.122	20.820	45.442	1.00	17.99	BTKB
ATOM	3154	O	VAL	529	42.673	21.120	44.381	1.00	19.19	BTKB
ATOM	3155	N	ASN	530	42.549	21.276	46.612	1.00	18.86	BTKB
ATOM	3156	CA	ASN	530	43.741	22.109	46.653	1.00	18.14	BTKB
ATOM	3157	CB	ASN	530	43.551	23.328	47.570	1.00	17.83	BTKB
ATOM	3158	CG	ASN	530	43.511	22.976	49.043	1.00	13.97	BTKB
ATOM	3159	OD1	ASN	530	43.831	21.862	49.446	1.00	14.33	BTKB
ATOM	3160	ND2	ASN	530	43.137	23.946	49.860	1.00	11.50	BTKB
ATOM	3161	C	ASN	530	44.977	21.294	47.024	1.00	17.68	BTKB
ATOM	3162	O	ASN	530	44.895	20.080	47.213	1.00	18.38	BTKB
ATOM	3163	N	ASP	531	46.119	21.964	47.104	1.00	20.29	BTKB
ATOM	3164	CA	ASP	531	47.392	21.329	47.433	1.00	24.52	BTKB
ATOM	3165	CB	ASP	531	48.498	22.388	47.520	1.00	26.76	BTKB
ATOM	3166	CG	ASP	531	47.956	23.787	47.753	1.00	26.59	BTKB
ATOM	3167	OD1	ASP	531	47.289	24.012	48.788	1.00	26.97	BTKB
ATOM	3168	OD2	ASP	531	48.180	24.652	46.879	1.00	28.82	BTKB
ATOM	3169	C	ASP	531	47.412	20.465	48.693	1.00	24.27	BTKB
ATOM	3170	O	ASP	531	48.269	19.596	48.838	1.00	28.06	BTKB
ATOM	3171	N	GLN	532	46.471	20.699	49.597	1.00	25.23	BTKB
ATOM	3172	CA	GLN	532	46.406	19.951	50.846	1.00	23.53	BTKB
ATOM	3173	CB	GLN	532	45.856	20.846	51.953	1.00	25.74	BTKB
ATOM	3174	CG	GLN	532	46.669	20.828	53.233	1.00	28.15	BTKB
ATOM	3175	CD	GLN	532	47.984	21.563	53.089	1.00	28.65	BTKB
ATOM	3176	OE1	GLN	532	48.062	22.769	53.342	1.00	29.05	BTKB
ATOM	3177	NE2	GLN	532	49.027	20.846	52.679	1.00	30.50	BTKB
ATOM	3178	C	GLN	532	45.556	18.686	50.772	1.00	22.38	BTKB
ATOM	3179	O	GLN	532	45.635	17.837	51.659	1.00	24.02	BTKB
ATOM	3180	N	GLY	533	44.751	18.557	49.722	1.00	18.67	BTKB
ATOM	3181	CA	GLY	533	43.877	17.402	49.601	1.00	13.49	BTKB
ATOM	3182	C	GLY	533	42.471	17.764	50.054	1.00	12.87	BTKB
ATOM	3183	O	GLY	533	41.574	16.915	50.094	1.00	13.75	BTKB

	Atom Number	Atom Type	Amino Acid Residue		X	Y	Z	Occ.	Temp Factor	
ATOM	3184	N	VAL	534	42.282	19.034	50.412	1.00	10.21	BTKB
ATOM	3185	CA	VAL	534	40.987	19.536	50.852	1.00	9.08	BTKB
ATOM	3186	CB	VAL	534	41.117	20.895	51.588	1.00	8.03	BTKB
ATOM	3187	CG1	VAL	534	39.739	21.465	51.918	1.00	9.23	BTKB
ATOM	3188	CG2	VAL	534	41.923	20.731	52.872	1.00	6.92	BTKB
ATOM	3189	C	VAL	534	40.062	19.712	49.655	1.00	8.68	BTKB
ATOM	3190	O	VAL	534	40.432	20.320	48.646	1.00	11.10	BTKB
ATOM	3191	N	VAL	535	38.860	19.158	49.777	1.00	10.57	BTKB
ATOM	3192	CA	VAL	535	37.848	19.239	48.732	1.00	9.29	BTKB
ATOM	3193	CB	VAL	535	37.058	17.918	48.622	1.00	8.60	BTKB
ATOM	3194	CG1	VAL	535	36.015	18.001	47.522	1.00	8.21	BTKB
ATOM	3195	CG2	VAL	535	38.002	16.776	48.351	1.00	4.73	BTKB
ATOM	3196	C	VAL	535	36.900	20.385	49.071	1.00	9.08	BTKB
ATOM	3197	O	VAL	535	36.415	20.493	50.200	1.00	9.32	BTKB
ATOM	3198	N	LYS	536	36.709	21.281	48.109	1.00	10.56	BTKB
ATOM	3199	CA	LYS	536	35.829	22.432	48.279	1.00	6.61	BTKB
ATOM	3200	CB	LYS	536	36.640	23.722	48.326	1.00	5.90	BTKB
ATOM	3201	CG	LYS	536	37.657	23.823	49.437	1.00	5.31	BTKB
ATOM	3202	CD	LYS	536	38.204	25.241	49.517	1.00	6.28	BTKB
ATOM	3203	CE	LYS	536	39.257	25.356	50.607	1.00	7.99	BTKB
ATOM	3204	NZ	LYS	536	39.577	26.769	50.898	1.00	2.74	BTKB
ATOM	3205	C	LYS	536	34.878	22.511	47.092	1.00	5.48	BTKB
ATOM	3206	O	LYS	536	35.288	22.309	45.942	1.00	3.48	BTKB
ATOM	3207	N	VAL	537	33.615	22.818	47.367	1.00	7.47	BTKB
ATOM	3208	CA	VAL	537	32.619	22.927	46.314	1.00	8.81	BTKB
ATOM	3209	CB	VAL	537	31.188	22.635	46.835	1.00	8.72	BTKB
ATOM	3210	CG1	VAL	537	30.952	23.324	48.142	1.00	11.64	BTKB
ATOM	3211	CG2	VAL	537	30.137	23.054	45.813	1.00	8.15	BTKB
ATOM	3212	C	VAL	537	32.700	24.273	45.616	1.00	9.66	BTKB
ATOM	3213	O	VAL	537	32.947	25.305	46.243	1.00	8.25	BTKB
ATOM	3214	N	SER	538	32.524	24.233	44.302	1.00	15.29	BTKB
ATOM	3215	CA	SER	538	32.588	25.410	43.456	1.00	20.41	BTKB
ATOM	3216	CB	SER	538	33.965	25.468	42.779	1.00	25.58	BTKB
ATOM	3217	OG	SER	538	34.210	26.711	42.133	1.00	28.06	BTKB
ATOM	3218	C	SER	538	31.478	25.310	42.407	1.00	20.96	BTKB
ATOM	3219	O	SER	538	30.516	24.555	42.573	1.00	20.92	BTKB
ATOM	3220	N	ASP	539	31.613	26.075	41.330	1.00	21.84	BTKB
ATOM	3221	CA	ASP	539	30.625	26.092	40.255	1.00	26.29	BTKB
ATOM	3222	CB	ASP	539	30.569	24.750	39.531	1.00	29.26	BTKB
ATOM	3223	CG	ASP	539	31.510	24.691	38.352	1.00	32.89	BTKB
ATOM	3224	OD1	ASP	539	31.014	24.523	37.217	1.00	32.96	BTKB
ATOM	3225	OD2	ASP	539	32.738	24.820	38.556	1.00	31.54	BTKB
ATOM	3226	C	ASP	539	29.236	26.497	40.719	1.00	25.45	BTKB
ATOM	3227	O	ASP	539	28.232	26.073	40.142	1.00	28.05	BTKB
ATOM	3228	N	PHE	540	29.187	27.276	41.793	1.00	23.51	BTKB
ATOM	3229	CA	PHE	540	27.931	27.777	42.318	1.00	22.85	BTKB
ATOM	3230	CB	PHE	540	27.860	27.612	43.846	1.00	17.06	BTKB
ATOM	3231	CG	PHE	540	28.988	28.269	44.586	1.00	14.42	BTKB
ATOM	3232	CD1	PHE	540	30.168	27.581	44.822	1.00	16.97	BTKB
ATOM	3233	CD2	PHE	540	28.878	29.583	45.030	1.00	16.54	BTKB
ATOM	3234	CE1	PHE	540	31.227	28.190	45.487	1.00	16.68	BTKB
ATOM	3235	CE2	PHE	540	29.928	30.197	45.694	1.00	17.48	BTKB
ATOM	3236	CZ	PHE	540	31.107	29.498	45.922	1.00	15.86	BTKB
ATOM	3237	C	PHE	540	27.912	29.244	41.902	1.00	24.94	BTKB
ATOM	3238	O	PHE	540	28.964	29.811	41.600	1.00	26.86	BTKB
ATOM	3239	N	GLY	541	26.733	29.849	41.844	1.00	25.65	BTKB
ATOM	3240	CA	GLY	541	26.643	31.243	41.437	1.00	30.15	BTKB
ATOM	3241	C	GLY	541	25.289	31.471	40.809	1.00	32.87	BTKB

	Atom Number	Atom Type	Amino Acid Residue		X	Y	Z	Occ.	Temp Factor	
ATOM	3242	O	GLY	541	24.421	32.123	41.387	1.00	34.13	BTKB
ATOM	3243	N	LEU	542	25.108	30.932	39.608	1.00	33.81	BTKB
ATOM	3244	CA	LEU	542	23.824	31.022	38.929	1.00	34.85	BTKB
ATOM	3245	CB	LEU	542	23.973	30.692	37.439	1.00	33.89	BTKB
ATOM	3246	CG	LEU	542	24.372	29.277	37.014	1.00	31.57	BTKB
ATOM	3247	CD1	LEU	542	23.136	28.530	36.552	1.00	30.77	BTKB
ATOM	3248	CD2	LEU	542	25.400	29.340	35.884	1.00	31.85	BTKB
ATOM	3249	C	LEU	542	22.935	29.998	39.648	1.00	36.33	BTKB
ATOM	3250	O	LEU	542	21.762	29.819	39.318	1.00	36.07	BTKB
ATOM	3251	N	SER	543	23.547	29.300	40.605	1.00	36.24	BTKB
ATOM	3252	CA	SER	543	22.895	28.316	41.450	1.00	34.49	BTKB
ATOM	3253	CB	SER	543	23.929	27.733	42.393	1.00	31.44	BTKB
ATOM	3254	OG	SER	543	25.053	27.284	41.653	1.00	26.36	BTKB
ATOM	3255	C	SER	543	21.837	29.077	42.230	1.00	36.96	BTKB
ATOM	3256	O	SER	543	22.137	30.058	42.908	1.00	39.90	BTKB
ATOM	3257	N	ARG	544	20.601	28.614	42.128	1.00	38.02	BTKB
ATOM	3258	CA	ARG	544	19.478	29.279	42.758	1.00	40.54	BTKB
ATOM	3259	CB	ARG	544	18.172	28.682	42.241	1.00	38.19	BTKB
ATOM	3260	CG	ARG	544	17.913	28.975	40.773	1.00	39.29	BTKB
ATOM	3261	CD	ARG	544	17.874	30.471	40.482	1.00	37.23	BTKB
ATOM	3262	NE	ARG	544	19.173	30.999	40.068	1.00	34.52	BTKB
ATOM	3263	CZ	ARG	544	19.810	32.003	40.668	1.00	33.10	BTKB
ATOM	3264	NH1	ARG	544	19.288	32.605	41.729	1.00	31.47	BTKB
ATOM	3265	NH2	ARG	544	20.965	32.431	40.183	1.00	33.04	BTKB
ATOM	3266	C	ARG	544	19.399	29.478	44.265	1.00	43.19	BTKB
ATOM	3267	O	ARG	544	20.208	28.975	45.047	1.00	41.34	BTKB
ATOM	3268	N	TYR	545	18.407	30.285	44.630	1.00	46.71	BTKB
ATOM	3269	CA	TYR	545	18.074	30.644	46.001	1.00	47.03	BTKB
ATOM	3270	CB	TYR	545	17.896	32.176	46.075	1.00	47.74	BTKB
ATOM	3271	CG	TYR	545	18.059	32.828	47.440	1.00	46.83	BTKB
ATOM	3272	CD1	TYR	545	17.606	32.210	48.606	1.00	47.23	BTKB
ATOM	3273	CE1	TYR	545	17.742	32.829	49.853	1.00	49.06	BTKB
ATOM	3274	CD2	TYR	545	18.653	34.085	47.557	1.00	48.20	BTKB
ATOM	3275	CE2	TYR	545	18.794	34.712	48.796	1.00	48.88	BTKB
ATOM	3276	CZ	TYR	545	18.338	34.080	49.937	1.00	48.87	BTKB
ATOM	3277	OH	TYR	545	18.491	34.695	51.158	1.00	49.33	BTKB
ATOM	3278	C	TYR	545	16.722	29.937	46.170	1.00	46.78	BTKB
ATOM	3279	O	TYR	545	16.490	28.886	45.570	1.00	46.40	BTKB
ATOM	3280	N	VAL	546	15.818	30.542	46.928	1.00	46.89	BTKB
ATOM	3281	CA	VAL	546	14.487	29.994	47.154	1.00	47.78	BTKB
ATOM	3282	CB	VAL	546	14.440	29.047	48.385	1.00	48.44	BTKB
ATOM	3283	CG1	VAL	546	15.047	27.696	48.038	1.00	49.26	BTKB
ATOM	3284	CG2	VAL	546	15.174	29.668	49.569	1.00	49.28	BTKB
ATOM	3285	C	VAL	546	13.555	31.180	47.374	1.00	47.25	BTKB
ATOM	3286	O	VAL	546	13.997	32.331	47.375	1.00	46.90	BTKB
ATOM	3287	N	LEU	547	12.269	30.908	47.546	1.00	47.06	BTKB
ATOM	3288	CA	LEU	547	11.291	31.964	47.764	1.00	47.07	BTKB
ATOM	3289	CB	LEU	547	10.767	32.492	46.419	1.00	46.14	BTKB
ATOM	3290	CG	LEU	547	9.916	33.768	46.428	1.00	46.13	BTKB
ATOM	3291	CD1	LEU	547	10.754	34.945	46.906	1.00	47.63	BTKB
ATOM	3292	CD2	LEU	547	9.359	34.035	45.035	1.00	47.76	BTKB
ATOM	3293	C	LEU	547	10.169	31.363	48.602	1.00	48.24	BTKB
ATOM	3294	O	LEU	547	10.439	30.733	49.623	1.00	48.69	BTKB
ATOM	3295	N	ASP	548	8.927	31.495	48.141	1.00	48.47	BTKB
ATOM	3296	CA	ASP	548	7.786	30.966	48.871	1.00	47.63	BTKB
ATOM	3297	CB	ASP	548	6.480	31.345	48.164	1.00	47.12	BTKB
ATOM	3298	CG	ASP	548	5.272	31.257	49.078	1.00	47.82	BTKB
ATOM	3299	OD1	ASP	548	4.251	30.681	48.653	1.00	47.08	BTKB

	Atom Number	Atom Type	Amino Acid Residue		X	Y	Z	Occ.	Temp Factor	
ATOM	3300	OD2	ASP	548	5.335	31.775	50.216	1.00	48.07	BTKB
ATOM	3301	C	ASP	548	7.907	29.451	49.017	1.00	46.66	BTKB
ATOM	3302	O	ASP	548	8.000	28.944	50.131	1.00	45.89	BTKB
ATOM	3303	N	ASP	549	7.954	28.735	47.896	1.00	47.04	BTKB
ATOM	3304	CA	ASP	549	8.064	27.278	47.937	1.00	45.92	BTKB
ATOM	3305	CB	ASP	549	6.683	26.643	48.100	1.00	44.19	BTKB
ATOM	3306	CG	ASP	549	6.155	26.745	49.517	1.00	43.52	BTKB
ATOM	3307	OD1	ASP	549	5.403	27.697	49.809	1.00	39.96	BTKB
ATOM	3308	OD2	ASP	549	6.494	25.870	50.340	1.00	43.98	BTKB
ATOM	3309	C	ASP	549	8.787	26.633	46.755	1.00	46.60	BTKB
ATOM	3310	O	ASP	549	9.179	25.470	46.835	1.00	48.82	BTKB
ATOM	3311	N	GLU	550	8.931	27.366	45.653	1.00	46.02	BTKB
ATOM	3312	CA	GLU	550	9.611	26.852	44.459	1.00	44.77	BTKB
ATOM	3313	CB	GLU	550	8.867	25.635	43.881	1.00	44.82	BTKB
ATOM	3314	CG	GLU	550	7.334	25.707	43.878	1.00	40.66	BTKB
ATOM	3315	CD	GLU	550	6.772	26.820	43.009	1.00	39.18	BTKB
ATOM	3316	OE1	GLU	550	6.074	27.701	43.554	1.00	38.17	BTKB
ATOM	3317	OE2	GLU	550	7.016	26.810	41.784	1.00	38.80	BTKB
ATOM	3318	C	GLU	550	9.775	27.931	43.389	1.00	45.63	BTKB
ATOM	3319	O	GLU	550	9.743	29.123	43.701	1.00	42.92	BTKB
ATOM	3320	N	TYR	551	9.969	27.509	42.141	1.00	45.07	BTKB
ATOM	3321	CA	TYR	551	10.119	28.427	41.016	1.00	46.80	BTKB
ATOM	3322	CB	TYR	551	11.410	29.243	41.147	1.00	47.58	BTKB
ATOM	3323	CG	TYR	551	12.684	28.433	41.176	1.00	46.34	BTKB
ATOM	3324	CD1	TYR	551	13.471	28.303	40.035	1.00	44.53	BTKB
ATOM	3325	CE1	TYR	551	14.668	27.596	40.063	1.00	45.32	BTKB
ATOM	3326	CD2	TYR	551	13.126	27.831	42.354	1.00	46.94	BTKB
ATOM	3327	CE2	TYR	551	14.324	27.120	42.394	1.00	46.70	BTKB
ATOM	3328	CZ	TYR	551	15.090	27.008	41.244	1.00	46.98	BTKB
ATOM	3329	OH	TYR	551	16.275	26.309	41.268	1.00	47.08	BTKB
ATOM	3330	C	TYR	551	10.061	27.697	39.665	1.00	47.92	BTKB
ATOM	3331	O	TYR	551	9.575	26.567	39.583	1.00	48.34	BTKB
ATOM	3332	N	THR	552	10.539	28.344	38.606	1.00	47.56	BTKB
ATOM	3333	CA	THR	552	10.519	27.736	37.279	1.00	47.33	BTKB
ATOM	3334	CB	THR	552	9.352	28.283	36.436	1.00	44.44	BTKB
ATOM	3335	OG1	THR	552	8.153	28.291	37.219	1.00	43.39	BTKB
ATOM	3336	CG2	THR	552	9.139	27.423	35.204	1.00	43.18	BTKB
ATOM	3337	C	THR	552	11.823	27.975	36.521	1.00	48.87	BTKB
ATOM	3338	O	THR	552	12.474	27.030	36.080	1.00	49.47	BTKB
ATOM	3339	N	SER	553	12.203	29.242	36.382	1.00	50.63	BTKB
ATOM	3340	CA	SER	553	13.425	29.614	35.674	1.00	51.18	BTKB
ATOM	3341	CB	SER	553	14.655	29.070	36.414	1.00	48.79	BTKB
ATOM	3342	OG	SER	553	14.750	29.635	37.713	1.00	43.88	BTKB
ATOM	3343	C	SER	553	13.395	29.148	34.210	1.00	51.91	BTKB
ATOM	3344	O	SER	553	12.331	29.148	33.584	1.00	52.66	BTKB
ATOM	3345	N	SER	554	14.552	28.772	33.667	1.00	50.57	BTKB
ATOM	3346	CA	SER	554	14.656	28.321	32.283	1.00	48.71	BTKB
ATOM	3347	CB	SER	554	16.121	28.056	31.928	1.00	49.93	BTKB
ATOM	3348	OG	SER	554	16.904	29.219	32.142	1.00	48.05	BTKB
ATOM	3349	C	SER	554	13.811	27.086	31.977	1.00	47.80	BTKB
ATOM	3350	O	SER	554	14.228	25.955	32.228	1.00	49.68	BTKB
ATOM	3351	N	VAL	555	12.624	27.319	31.427	1.00	45.84	BTKB
ATOM	3352	CA	VAL	555	11.702	26.247	31.067	1.00	42.92	BTKB
ATOM	3353	CB	VAL	555	10.362	26.821	30.570	1.00	38.45	BTKB
ATOM	3354	CG1	VAL	555	9.363	25.703	30.345	1.00	41.05	BTKB
ATOM	3355	CG2	VAL	555	9.819	27.822	31.577	1.00	38.78	BTKB
ATOM	3356	C	VAL	555	12.319	25.381	29.969	1.00	43.08	BTKB
ATOM	3357	O	VAL	555	12.798	25.904	28.963	1.00	45.11	BTKB

	Atom Number	Atom Type	Amino Acid Residue		X	Y	Z	Occ.	Temp Factor	
ATOM	3358	N	GLY	556	12.284	24.062	30.157	1.00	40.17	BTKB
ATOM	3359	CA	GLY	556	12.860	23.144	29.185	1.00	36.28	BTKB
ATOM	3360	C	GLY	556	14.375	23.211	29.259	1.00	34.46	BTKB
ATOM	3361	O	GLY	556	14.937	24.302	29.258	1.00	34.17	BTKB
ATOM	3362	N	SER	557	15.042	22.065	29.357	1.00	37.09	BTKB
ATOM	3363	CA	SER	557	16.501	22.047	29.451	1.00	39.60	BTKB
ATOM	3364	CB	SER	557	16.959	22.896	30.650	1.00	42.29	BTKB
ATOM	3365	OG	SER	557	18.341	23.216	30.573	1.00	42.78	BTKB
ATOM	3366	C	SER	557	17.084	20.634	29.581	1.00	39.69	BTKB
ATOM	3367	O	SER	557	16.355	19.635	29.559	1.00	37.28	BTKB
ATOM	3368	N	LYS	558	18.408	20.572	29.710	1.00	38.88	BTKB
ATOM	3369	CA	LYS	558	19.131	19.317	29.861	1.00	38.70	BTKB
ATOM	3370	CB	LYS	558	20.122	19.107	28.711	1.00	40.51	BTKB
ATOM	3371	CG	LYS	558	19.507	19.185	27.328	1.00	39.86	BTKB
ATOM	3372	CD	LYS	558	19.318	20.630	26.895	1.00	40.70	BTKB
ATOM	3373	CE	LYS	558	18.358	20.719	25.736	1.00	38.88	BTKB
ATOM	3374	NZ	LYS	558	17.034	20.178	26.138	1.00	36.01	BTKB
ATOM	3375	C	LYS	558	19.883	19.350	31.188	1.00	38.02	BTKB
ATOM	3376	O	LYS	558	20.904	20.019	31.327	1.00	38.61	BTKB
ATOM	3377	N	PHE	559	19.342	18.648	32.171	1.00	35.11	BTKB
ATOM	3378	CA	PHE	559	19.935	18.570	33.499	1.00	32.80	BTKB
ATOM	3379	CB	PHE	559	18.836	18.268	34.530	1.00	35.42	BTKB
ATOM	3380	CG	PHE	559	17.431	18.422	33.991	1.00	38.43	BTKB
ATOM	3381	CD1	PHE	559	16.647	17.302	33.728	1.00	35.87	BTKB
ATOM	3382	CD2	PHE	559	16.902	19.685	33.730	1.00	35.45	BTKB
ATOM	3383	CE1	PHE	559	15.360	17.434	33.212	1.00	38.06	BTKB
ATOM	3384	CE2	PHE	559	15.616	19.827	33.214	1.00	33.30	BTKB
ATOM	3385	CZ	PHE	559	14.843	18.696	32.954	1.00	36.08	BTKB
ATOM	3386	C	PHE	559	20.947	17.423	33.473	1.00	30.75	BTKB
ATOM	3387	O	PHE	559	20.919	16.597	32.556	1.00	30.59	BTKB
ATOM	3388	N	PRO	560	21.843	17.341	34.478	1.00	27.32	BTKB
ATOM	3389	CD	PRO	560	22.005	18.208	35.658	1.00	23.09	BTKB
ATOM	3390	CA	PRO	560	22.832	16.255	34.503	1.00	23.53	BTKB
ATOM	3391	CB	PRO	560	23.640	16.561	35.765	1.00	20.79	BTKB
ATOM	3392	CG	PRO	560	22.668	17.275	36.631	1.00	19.96	BTKB
ATOM	3393	C	PRO	560	22.166	14.872	34.563	1.00	23.08	BTKB
ATOM	3394	O	PRO	560	22.778	13.857	34.212	1.00	21.72	BTKB
ATOM	3395	N	VAL	561	20.921	14.846	35.037	1.00	22.54	BTKB
ATOM	3396	CA	VAL	561	20.118	13.629	35.138	1.00	21.12	BTKB
ATOM	3397	CB	VAL	561	20.065	12.847	33.786	1.00	24.08	BTKB
ATOM	3398	CG1	VAL	561	19.095	11.656	33.890	1.00	22.39	BTKB
ATOM	3399	CG2	VAL	561	19.654	13.778	32.641	1.00	24.23	BTKB
ATOM	3400	C	VAL	561	20.510	12.666	36.259	1.00	18.16	BTKB
ATOM	3401	O	VAL	561	19.709	12.404	37.162	1.00	18.62	BTKB
ATOM	3402	N	ARG	562	21.729	12.141	36.210	1.00	13.44	BTKB
ATOM	3403	CA	ARG	562	22.182	11.192	37.221	1.00	14.89	BTKB
ATOM	3404	CB	ARG	562	23.606	10.726	36.919	1.00	18.46	BTKB
ATOM	3405	CG	ARG	562	23.764	9.858	35.677	1.00	20.23	BTKB
ATOM	3406	CD	ARG	562	23.654	10.637	34.387	1.00	19.70	BTKB
ATOM	3407	NE	ARG	562	24.262	9.895	33.284	1.00	26.34	BTKB
ATOM	3408	CZ	ARG	562	23.614	9.045	32.495	1.00	23.35	BTKB
ATOM	3409	NH1	ARG	562	22.320	8.821	32.670	1.00	25.49	BTKB
ATOM	3410	NH2	ARG	562	24.277	8.394	31.549	1.00	20.77	BTKB
ATOM	3411	C	ARG	562	22.129	11.748	38.639	1.00	14.76	BTKB
ATOM	3412	O	ARG	562	21.745	11.051	39.584	1.00	15.25	BTKB
ATOM	3413	N	TRP	563	22.510	13.012	38.769	1.00	13.56	BTKB
ATOM	3414	CA	TRP	563	22.544	13.707	40.050	1.00	15.17	BTKB
ATOM	3415	CB	TRP	563	23.680	14.733	40.021	1.00	17.58	BTKB

	Atom Number	Atom Type	Amino Acid Residue		X	Y	Z	Occ.	Temp Factor	
ATOM	3416	CG	TRP	563	25.024	14.120	39.845	1.00	16.68	BTKB
ATOM	3417	CD2	TRP	563	25.614	13.658	38.619	1.00	18.94	BTKB
ATOM	3418	CE2	TRP	563	26.870	13.106	38.945	1.00	19.94	BTKB
ATOM	3419	CE3	TRP	563	25.202	13.651	37.280	1.00	18.43	BTKB
ATOM	3420	CD1	TRP	563	25.924	13.848	40.830	1.00	12.29	BTKB
ATOM	3421	NE1	TRP	563	27.028	13.233	40.300	1.00	18.47	BTKB
ATOM	3422	CZ2	TRP	563	27.724	12.552	37.979	1.00	20.36	BTKB
ATOM	3423	CZ3	TRP	563	26.056	13.097	36.314	1.00	17.95	BTKB
ATOM	3424	CH2	TRP	563	27.298	12.555	36.674	1.00	17.39	BTKB
ATOM	3425	C	TRP	563	21.236	14.431	40.346	1.00	16.25	BTKB
ATOM	3426	O	TRP	563	21.202	15.361	41.157	1.00	15.08	BTKB
ATOM	3427	N	SER	564	20.153	13.979	39.728	1.00	16.15	BTKB
ATOM	3428	CA	SER	564	18.877	14.647	39.894	1.00	15.25	BTKB
ATOM	3429	CB	SER	564	18.450	15.226	38.540	1.00	12.15	BTKB
ATOM	3430	OG	SER	564	19.456	16.046	37.961	1.00	15.22	BTKB
ATOM	3431	C	SER	564	17.732	13.812	40.466	1.00	18.06	BTKB
ATOM	3432	O	SER	564	17.643	12.604	40.245	1.00	18.41	BTKB
ATOM	3433	N	PRO	565	16.852	14.453	41.250	1.00	19.48	BTKB
ATOM	3434	CD	PRO	565	17.013	15.807	41.805	1.00	16.11	BTKB
ATOM	3435	CA	PRO	565	15.699	13.784	41.854	1.00	20.89	BTKB
ATOM	3436	CB	PRO	565	15.154	14.852	42.801	1.00	20.19	BTKB
ATOM	3437	CG	PRO	565	16.331	15.681	43.117	1.00	16.32	BTKB
ATOM	3438	C	PRO	565	14.678	13.499	40.748	1.00	24.06	BTKB
ATOM	3439	O	PRO	565	14.578	14.260	39.778	1.00	25.01	BTKB
ATOM	3440	N	PRO	566	13.878	12.433	40.892	1.00	25.49	BTKB
ATOM	3441	CD	PRO	566	13.859	11.410	41.947	1.00	24.25	BTKB
ATOM	3442	CA	PRO	566	12.887	12.126	39.853	1.00	27.84	BTKB
ATOM	3443	CB	PRO	566	12.114	10.966	40.470	1.00	26.01	BTKB
ATOM	3444	CG	PRO	566	13.169	10.267	41.256	1.00	28.12	BTKB
ATOM	3445	C	PRO	566	11.985	13.330	39.585	1.00	29.05	BTKB
ATOM	3446	O	PRO	566	11.516	13.537	38.465	1.00	31.25	BTKB
ATOM	3447	N	GLU	567	11.805	14.151	40.613	1.00	30.57	BTKB
ATOM	3448	CA	GLU	567	10.982	15.348	40.518	1.00	31.66	BTKB
ATOM	3449	CB	GLU	567	11.006	16.119	41.841	1.00	30.30	BTKB
ATOM	3450	CG	GLU	567	10.491	15.346	43.051	1.00	31.92	BTKB
ATOM	3451	CD	GLU	567	11.493	14.337	43.594	1.00	30.79	BTKB
ATOM	3452	OE1	GLU	567	12.348	14.722	44.424	1.00	29.93	BTKB
ATOM	3453	OE2	GLU	567	11.412	13.156	43.200	1.00	33.30	BTKB
ATOM	3454	C	GLU	567	11.483	16.253	39.394	1.00	29.70	BTKB
ATOM	3455	O	GLU	567	10.723	16.629	38.494	1.00	30.08	BTKB
ATOM	3456	N	VAL	568	12.779	16.553	39.421	1.00	30.70	BTKB
ATOM	3457	CA	VAL	568	13.382	17.422	38.419	1.00	30.50	BTKB
ATOM	3458	CB	VAL	568	14.737	17.976	38.885	1.00	30.30	BTKB
ATOM	3459	CG1	VAL	568	14.584	18.738	40.177	1.00	28.02	BTKB
ATOM	3460	CG2	VAL	568	15.718	16.866	39.048	1.00	24.92	BTKB
ATOM	3461	C	VAL	568	13.553	16.767	37.052	1.00	31.05	BTKB
ATOM	3462	O	VAL	568	13.494	17.444	36.028	1.00	33.18	BTKB
ATOM	3463	N	LEU	569	13.746	15.454	37.039	1.00	33.44	BTKB
ATOM	3464	CA	LEU	569	13.924	14.711	35.791	1.00	34.63	BTKB
ATOM	3465	CB	LEU	569	14.322	13.266	36.091	1.00	32.99	BTKB
ATOM	3466	CG	LEU	569	15.657	13.167	36.828	1.00	31.76	BTKB
ATOM	3467	CD1	LEU	569	15.945	11.733	37.268	1.00	26.25	BTKB
ATOM	3468	CD2	LEU	569	16.742	13.705	35.902	1.00	28.56	BTKB
ATOM	3469	C	LEU	569	12.687	14.733	34.899	1.00	36.45	BTKB
ATOM	3470	O	LEU	569	12.741	14.313	33.745	1.00	36.82	BTKB
ATOM	3471	N	MET	570	11.568	15.192	35.451	1.00	39.88	BTKB
ATOM	3472	CA	MET	570	10.325	15.276	34.700	1.00	39.46	BTKB
ATOM	3473	CB	MET	570	9.255	14.381	35.332	1.00	39.18	BTKB

	Atom Number	Atom Type	Amino Acid Residue		X	Y	Z	Occ.	Temp Factor	
ATOM	3474	CG	MET	570	9.607	12.895	35.325	1.00	38.41	BTKB
ATOM	3475	SD	MET	570	8.311	11.837	36.007	1.00	37.44	BTKB
ATOM	3476	CE	MET	570	8.698	11.878	37.754	1.00	37.14	BTKB
ATOM	3477	C	MET	570	9.831	16.719	34.592	1.00	40.77	BTKB
ATOM	3478	O	MET	570	9.802	17.287	33.499	1.00	41.26	BTKB
ATOM	3479	N	TYR	571	9.493	17.327	35.727	1.00	42.07	BTKB
ATOM	3480	CA	TYR	571	8.985	18.703	35.739	1.00	43.90	BTKB
ATOM	3481	CB	TYR	571	7.560	18.741	36.322	1.00	44.93	BTKB
ATOM	3482	CG	TYR	571	7.386	17.933	37.593	1.00	45.07	BTKB
ATOM	3483	CD1	TYR	571	6.986	16.595	37.542	1.00	45.70	BTKB
ATOM	3484	CE1	TYR	571	6.863	15.833	38.706	1.00	46.81	BTKB
ATOM	3485	CD2	TYR	571	7.653	18.493	38.842	1.00	46.94	BTKB
ATOM	3486	CE2	TYR	571	7.531	17.740	40.011	1.00	46.48	BTKB
ATOM	3487	CZ	TYR	571	7.139	16.412	39.937	1.00	46.81	BTKB
ATOM	3488	OH	TYR	571	7.043	15.662	41.089	1.00	45.30	BTKB
ATOM	3489	C	TYR	571	9.886	19.698	36.469	1.00	42.72	BTKB
ATOM	3490	O	TYR	571	9.411	20.690	37.014	1.00	42.57	BTKB
ATOM	3491	N	SER	572	11.183	19.410	36.490	1.00	42.42	BTKB
ATOM	3492	CA	SER	572	12.181	20.260	37.136	1.00	40.33	BTKB
ATOM	3493	CB	SER	572	12.616	21.368	36.175	1.00	41.33	BTKB
ATOM	3494	OG	SER	572	13.136	20.813	34.978	1.00	43.33	BTKB
ATOM	3495	C	SER	572	11.803	20.849	38.500	1.00	37.82	BTKB
ATOM	3496	O	SER	572	11.843	22.062	38.693	1.00	36.53	BTKB
ATOM	3497	N	LYS	573	11.481	19.980	39.454	1.00	36.19	BTKB
ATOM	3498	CA	LYS	573	11.116	20.421	40.798	1.00	34.19	BTKB
ATOM	3499	CB	LYS	573	10.084	19.476	41.406	1.00	31.01	BTKB
ATOM	3500	CG	LYS	573	9.519	19.960	42.718	1.00	33.03	BTKB
ATOM	3501	CD	LYS	573	8.828	21.296	42.551	1.00	26.52	BTKB
ATOM	3502	CE	LYS	573	9.322	22.299	43.578	1.00	24.03	BTKB
ATOM	3503	NZ	LYS	573	10.709	22.745	43.291	1.00	17.04	BTKB
ATOM	3504	C	LYS	573	12.335	20.550	41.720	1.00	35.59	BTKB
ATOM	3505	O	LYS	573	12.666	19.636	42.481	1.00	33.63	BTKB
ATOM	3506	N	PHE	574	13.001	21.696	41.620	1.00	38.79	BTKB
ATOM	3507	CA	PHE	574	14.198	22.030	42.404	1.00	36.81	BTKB
ATOM	3508	CB	PHE	574	15.061	23.057	41.657	1.00	37.78	BTKB
ATOM	3509	CG	PHE	574	14.330	23.776	40.555	1.00	36.05	BTKB
ATOM	3510	CD1	PHE	574	13.099	24.384	40.792	1.00	37.69	BTKB
ATOM	3511	CD2	PHE	574	14.856	23.811	39.269	1.00	38.01	BTKB
ATOM	3512	CE1	PHE	574	12.405	25.007	39.768	1.00	37.96	BTKB
ATOM	3513	CE2	PHE	574	14.168	24.435	38.236	1.00	38.31	BTKB
ATOM	3514	CZ	PHE	574	12.938	25.034	38.487	1.00	39.59	BTKB
ATOM	3515	C	PHE	574	13.865	22.573	43.785	1.00	34.93	BTKB
ATOM	3516	O	PHE	574	13.125	23.546	43.917	1.00	35.39	BTKB
ATOM	3517	N	SER	575	14.473	21.988	44.806	1.00	32.93	BTKB
ATOM	3518	CA	SER	575	14.229	22.405	46.178	1.00	31.78	BTKB
ATOM	3519	CB	SER	575	13.053	21.607	46.740	1.00	30.36	BTKB
ATOM	3520	OG	SER	575	13.264	20.216	46.563	1.00	31.46	BTKB
ATOM	3521	C	SER	575	15.459	22.157	47.040	1.00	32.41	BTKB
ATOM	3522	O	SER	575	16.492	21.704	46.542	1.00	32.95	BTKB
ATOM	3523	N	SER	576	15.338	22.453	48.333	1.00	31.52	BTKB
ATOM	3524	CA	SER	576	16.414	22.242	49.297	1.00	26.86	BTKB
ATOM	3525	CB	SER	576	15.917	22.607	50.695	1.00	30.38	BTKB
ATOM	3526	OG	SER	576	14.621	22.070	50.923	1.00	33.61	BTKB
ATOM	3527	C	SER	576	16.827	20.772	49.275	1.00	23.09	BTKB
ATOM	3528	O	SER	576	18.003	20.432	49.457	1.00	18.87	BTKB
ATOM	3529	N	LYS	577	15.840	19.913	49.036	1.00	19.70	BTKB
ATOM	3530	CA	LYS	577	16.048	18.477	48.973	1.00	15.88	BTKB
ATOM	3531	CB	LYS	577	14.753	17.732	49.286	1.00	15.45	BTKB

Atom Number	Atom Type	Amino Acid Residue		X	Y	Z	Occ.	Temp Factor	
ATOM 3532	CG	LYS	577	14.598	17.347	50.748	1.00	14.36	BTKB
ATOM 3533	CD	LYS	577	14.604	18.548	51.663	1.00	10.74	BTKB
ATOM 3534	CE	LYS	577	14.692	18.116	53.102	1.00	8.91	BTKB
ATOM 3535	NZ	LYS	577	15.888	17.272	53.339	1.00	13.99	BTKB
ATOM 3536	C	LYS	577	16.627	17.985	47.659	1.00	15.31	BTKB
ATOM 3537	O	LYS	577	16.966	16.815	47.550	1.00	18.88	BTKB
ATOM 3538	N	SER	578	16.737	18.855	46.660	1.00	15.22	BTKB
ATOM 3539	CA	SER	578	17.316	18.453	45.382	1.00	14.59	BTKB
ATOM 3540	CB	SER	578	17.043	19.491	44.290	1.00	18.56	BTKB
ATOM 3541	OG	SER	578	15.680	19.499	43.903	1.00	23.33	BTKB
ATOM 3542	C	SER	578	18.821	18.282	45.557	1.00	15.07	BTKB
ATOM 3543	O	SER	578	19.398	17.307	45.075	1.00	16.57	BTKB
ATOM 3544	N	ASP	579	19.448	19.220	46.267	1.00	15.79	BTKB
ATOM 3545	CA	ASP	579	20.888	19.162	46.517	1.00	15.96	BTKB
ATOM 3546	CB	ASP	579	21.387	20.432	47.217	1.00	15.23	BTKB
ATOM 3547	CG	ASP	579	21.587	21.610	46.261	1.00	16.89	BTKB
ATOM 3548	OD1	ASP	579	21.403	22.748	46.724	1.00	14.46	BTKB
ATOM 3549	OD2	ASP	579	21.953	21.414	45.075	1.00	17.09	BTKB
ATOM 3550	C	ASP	579	21.218	17.955	47.378	1.00	18.59	BTKB
ATOM 3551	O	ASP	579	22.329	17.422	47.313	1.00	20.19	BTKB
ATOM 3552	N	ILE	580	20.255	17.532	48.194	1.00	18.03	BTKB
ATOM 3553	CA	ILE	580	20.447	16.373	49.054	1.00	17.50	BTKB
ATOM 3554	CB	ILE	580	19.272	16.189	50.035	1.00	15.12	BTKB
ATOM 3555	CG2	ILE	580	19.377	14.837	50.760	1.00	14.16	BTKB
ATOM 3556	CG1	ILE	580	19.274	17.327	51.057	1.00	13.57	BTKB
ATOM 3557	CD	ILE	580	20.508	17.347	51.943	1.00	12.21	BTKB
ATOM 3558	C	ILE	580	20.620	15.127	48.193	1.00	19.53	BTKB
ATOM 3559	O	ILE	580	21.548	14.353	48.411	1.00	26.22	BTKB
ATOM 3560	N	TRP	581	19.754	14.960	47.194	1.00	16.88	BTKB
ATOM 3561	CA	TRP	581	19.838	13.815	46.291	1.00	11.89	BTKB
ATOM 3562	CB	TRP	581	18.753	13.885	45.217	1.00	8.40	BTKB
ATOM 3563	CG	TRP	581	18.746	12.692	44.284	1.00	7.47	BTKB
ATOM 3564	CD2	TRP	581	17.741	11.675	44.201	1.00	6.04	BTKB
ATOM 3565	CE2	TRP	581	18.130	10.788	43.165	1.00	6.60	BTKB
ATOM 3566	CE3	TRP	581	16.547	11.429	44.890	1.00	9.89	BTKB
ATOM 3567	CD1	TRP	581	19.675	12.386	43.329	1.00	5.91	BTKB
ATOM 3568	NE1	TRP	581	19.310	11.247	42.654	1.00	4.72	BTKB
ATOM 3569	CZ2	TRP	581	17.362	9.676	42.805	1.00	7.81	BTKB
ATOM 3570	CZ3	TRP	581	15.783	10.324	44.532	1.00	6.46	BTKB
ATOM 3571	CH2	TRP	581	16.195	9.462	43.498	1.00	13.07	BTKB
ATOM 3572	C	TRP	581	21.206	13.785	45.625	1.00	10.29	BTKB
ATOM 3573	O	TRP	581	21.909	12.770	45.678	1.00	11.92	BTKB
ATOM 3574	N	ALA	582	21.590	14.911	45.022	1.00	10.55	BTKB
ATOM 3575	CA	ALA	582	22.872	15.023	44.341	1.00	4.48	BTKB
ATOM 3576	CB	ALA	582	23.003	16.387	43.684	1.00	4.04	BTKB
ATOM 3577	C	ALA	582	24.058	14.758	45.261	1.00	6.67	BTKB
ATOM 3578	O	ALA	582	25.056	14.185	44.835	1.00	8.34	BTKB
ATOM 3579	N	PHE	583	23.943	15.132	46.531	1.00	9.39	BTKB
ATOM 3580	CA	PHE	583	25.038	14.908	47.478	1.00	8.21	BTKB
ATOM 3581	CB	PHE	583	24.742	15.558	48.833	1.00	10.48	BTKB
ATOM 3582	CG	PHE	583	25.754	15.223	49.901	1.00	8.42	BTKB
ATOM 3583	CD1	PHE	583	27.045	15.745	49.847	1.00	7.25	BTKB
ATOM 3584	CD2	PHE	583	25.425	14.361	50.936	1.00	7.08	BTKB
ATOM 3585	CE1	PHE	583	27.995	15.408	50.807	1.00	4.56	BTKB
ATOM 3586	CE2	PHE	583	26.361	14.020	51.895	1.00	6.14	BTKB
ATOM 3587	CZ	PHE	583	27.654	14.543	51.830	1.00	8.80	BTKB
ATOM 3588	C	PHE	583	25.295	13.424	47.682	1.00	9.03	BTKB
ATOM 3589	O	PHE	583	26.435	13.005	47.927	1.00	3.30	BTKB

	Atom Number	Atom Type	Amino Acid Residue		X	Y	Z	Occ.	Temp Factor	
ATOM	3590	N	GLY	584	24.225	12.640	47.618	1.00	10.23	BTKB
ATOM	3591	CA	GLY	584	24.340	11.203	47.786	1.00	9.17	BTKB
ATOM	3592	C	GLY	584	25.042	10.597	46.593	1.00	7.39	BTKB
ATOM	3593	O	GLY	584	25.857	9.690	46.735	1.00	10.68	BTKB
ATOM	3594	N	VAL	585	24.728	11.112	45.408	1.00	9.02	BTKB
ATOM	3595	CA	VAL	585	25.350	10.624	44.186	1.00	7.71	BTKB
ATOM	3596	CB	VAL	585	24.658	11.184	42.925	1.00	6.04	BTKB
ATOM	3597	CG1	VAL	585	25.359	10.699	41.669	1.00	4.31	BTKB
ATOM	3598	CG2	VAL	585	23.208	10.747	42.896	1.00	6.37	BTKB
ATOM	3599	C	VAL	585	26.818	11.010	44.211	1.00	7.83	BTKB
ATOM	3600	O	VAL	585	27.665	10.264	43.720	1.00	10.87	BTKB
ATOM	3601	N	LEU	586	27.112	12.183	44.778	1.00	7.00	BTKB
ATOM	3602	CA	LEU	586	28.484	12.670	44.899	1.00	4.53	BTKB
ATOM	3603	CB	LEU	586	28.522	14.102	45.455	1.00	2.00	BTKB
ATOM	3604	CG	LEU	586	29.880	14.670	45.894	1.00	2.12	BTKB
ATOM	3605	CD1	LEU	586	30.010	16.106	45.440	1.00	7.20	BTKB
ATOM	3606	CD2	LEU	586	30.029	14.602	47.413	1.00	4.41	BTKB
ATOM	3607	C	LEU	586	29.247	11.724	45.812	1.00	5.96	BTKB
ATOM	3608	O	LEU	586	30.365	11.323	45.493	1.00	8.74	BTKB
ATOM	3609	N	MET	587	28.625	11.339	46.924	1.00	6.85	BTKB
ATOM	3610	CA	MET	587	29.250	10.419	47.872	1.00	8.03	BTKB
ATOM	3611	CB	MET	587	28.314	10.108	49.042	1.00	7.46	BTKB
ATOM	3612	CG	MET	587	28.255	11.188	50.097	1.00	11.21	BTKB
ATOM	3613	SD	MET	587	27.548	10.557	51.621	1.00	9.37	BTKB
ATOM	3614	CE	MET	587	25.884	10.932	51.370	1.00	7.42	BTKB
ATOM	3615	C	MET	587	29.559	9.139	47.130	1.00	8.01	BTKB
ATOM	3616	O	MET	587	30.618	8.534	47.314	1.00	9.09	BTKB
ATOM	3617	N	TRP	588	28.613	8.733	46.290	1.00	6.67	BTKB
ATOM	3618	CA	TRP	588	28.754	7.532	45.484	1.00	4.52	BTKB
ATOM	3619	CB	TRP	588	27.460	7.282	44.706	1.00	2.40	BTKB
ATOM	3620	CG	TRP	588	27.421	5.979	44.025	1.00	4.75	BTKB
ATOM	3621	CD2	TRP	588	27.806	5.713	42.674	1.00	7.11	BTKB
ATOM	3622	CE2	TRP	588	27.660	4.323	42.468	1.00	6.92	BTKB
ATOM	3623	CE3	TRP	588	28.264	6.509	41.618	1.00	8.00	BTKB
ATOM	3624	CD1	TRP	588	27.059	4.787	44.566	1.00	4.69	BTKB
ATOM	3625	NE1	TRP	588	27.204	3.786	43.641	1.00	6.93	BTKB
ATOM	3626	CZ2	TRP	588	27.956	3.711	41.252	1.00	11.08	BTKB
ATOM	3627	CZ3	TRP	588	28.563	5.904	40.409	1.00	10.43	BTKB
ATOM	3628	CH2	TRP	588	28.406	4.511	40.235	1.00	14.47	BTKB
ATOM	3629	C	TRP	588	29.955	7.700	44.542	1.00	5.71	BTKB
ATOM	3630	O	TRP	588	30.785	6.780	44.407	1.00	2.00	BTKB
ATOM	3631	N	GLU	589	30.085	8.893	43.951	1.00	6.18	BTKB
ATOM	3632	CA	GLU	589	31.198	9.194	43.050	1.00	9.53	BTKB
ATOM	3633	CB	GLU	589	31.105	10.614	42.497	1.00	6.96	BTKB
ATOM	3634	CG	GLU	589	29.917	10.879	41.608	1.00	10.53	BTKB
ATOM	3635	CD	GLU	589	29.935	12.283	41.037	1.00	10.94	BTKB
ATOM	3636	OE1	GLU	589	29.344	13.189	41.665	1.00	11.25	BTKB
ATOM	3637	OE2	GLU	589	30.537	12.479	39.959	1.00	15.70	BTKB
ATOM	3638	C	GLU	589	32.507	9.070	43.823	1.00	11.10	BTKB
ATOM	3639	O	GLU	589	33.519	8.622	43.280	1.00	15.09	BTKB
ATOM	3640	N	ILE	590	32.485	9.475	45.087	1.00	9.46	BTKB
ATOM	3641	CA	ILE	590	33.668	9.413	45.928	1.00	8.87	BTKB
ATOM	3642	CB	ILE	590	33.453	10.208	47.246	1.00	3.55	BTKB
ATOM	3643	CG2	ILE	590	34.623	10.013	48.187	1.00	2.00	BTKB
ATOM	3644	CG1	ILE	590	33.296	11.696	46.913	1.00	2.10	BTKB
ATOM	3645	CD	ILE	590	32.967	12.585	48.066	1.00	2.00	BTKB
ATOM	3646	C	ILE	590	34.078	7.960	46.194	1.00	12.45	BTKB
ATOM	3647	O	ILE	590	35.167	7.525	45.780	1.00	11.72	BTKB

	Atom Number	Atom Type	Amino Acid Residue		X	Y	Z	Occ.	Temp Factor	
ATOM	3648	N	TYR	591	33.184	7.192	46.816	1.00	15.34	BTKB
ATOM	3649	CA	TYR	591	33.461	5.791	47.111	1.00	13.05	BTKB
ATOM	3650	CB	TYR	591	32.425	5.230	48.090	1.00	12.55	BTKB
ATOM	3651	CG	TYR	591	32.669	5.737	49.488	1.00	10.68	BTKB
ATOM	3652	CD1	TYR	591	32.075	6.918	49.936	1.00	9.88	BTKB
ATOM	3653	CE1	TYR	591	32.415	7.474	51.175	1.00	8.76	BTKB
ATOM	3654	CD2	TYR	591	33.598	5.110	50.321	1.00	13.54	BTKB
ATOM	3655	CE2	TYR	591	33.940	5.653	51.564	1.00	10.89	BTKB
ATOM	3656	CZ	TYR	591	33.349	6.836	51.978	1.00	9.81	BTKB
ATOM	3657	OH	TYR	591	33.712	7.402	53.171	1.00	9.51	BTKB
ATOM	3658	C	TYR	591	33.585	4.938	45.850	1.00	12.23	BTKB
ATOM	3659	O	TYR	591	34.024	3.790	45.909	1.00	17.98	BTKB
ATOM	3660	N	SER	592	33.185	5.499	44.713	1.00	11.77	BTKB
ATOM	3661	CA	SER	592	33.290	4.803	43.438	1.00	11.46	BTKB
ATOM	3662	CB	SER	592	32.104	5.134	42.543	1.00	9.01	BTKB
ATOM	3663	OG	SER	592	30.947	4.504	43.038	1.00	12.06	BTKB
ATOM	3664	C	SER	592	34.589	5.180	42.739	1.00	12.26	BTKB
ATOM	3665	O	SER	592	34.888	4.685	41.654	1.00	11.21	BTKB
ATOM	3666	N	LEU	593	35.342	6.075	43.367	1.00	11.73	BTKB
ATOM	3667	CA	LEU	593	36.608	6.528	42.835	1.00	13.65	BTKB
ATOM	3668	CB	LEU	593	37.646	5.408	42.919	1.00	14.04	BTKB
ATOM	3669	CG	LEU	593	38.563	5.446	44.143	1.00	15.85	BTKB
ATOM	3670	CD1	LEU	593	37.764	5.702	45.398	1.00	12.60	BTKB
ATOM	3671	CD2	LEU	593	39.346	4.161	44.251	1.00	12.99	BTKB
ATOM	3672	C	LEU	593	36.494	7.086	41.422	1.00	14.18	BTKB
ATOM	3673	O	LEU	593	37.319	6.795	40.554	1.00	16.11	BTKB
ATOM	3674	N	GLY	594	35.464	7.899	41.200	1.00	14.51	BTKB
ATOM	3675	CA	GLY	594	35.274	8.508	39.897	1.00	13.72	BTKB
ATOM	3676	C	GLY	594	34.316	7.825	38.946	1.00	14.52	BTKB
ATOM	3677	O	GLY	594	34.060	8.347	37.868	1.00	16.91	BTKB
ATOM	3678	N	LYS	595	33.794	6.662	39.321	1.00	13.58	BTKB
ATOM	3679	CA	LYS	595	32.846	5.947	38.470	1.00	13.97	BTKB
ATOM	3680	CB	LYS	595	32.358	4.663	39.138	1.00	13.75	BTKB
ATOM	3681	CG	LYS	595	33.049	3.412	38.664	1.00	13.60	BTKB
ATOM	3682	CD	LYS	595	32.338	2.180	39.200	1.00	17.92	BTKB
ATOM	3683	CE	LYS	595	32.493	2.037	40.711	1.00	17.12	BTKB
ATOM	3684	NZ	LYS	595	31.791	0.819	41.230	1.00	20.68	BTKB
ATOM	3685	C	LYS	595	31.644	6.812	38.144	1.00	14.65	BTKB
ATOM	3686	O	LYS	595	31.032	7.404	39.031	1.00	17.03	BTKB
ATOM	3687	N	MET	596	31.300	6.865	36.866	1.00	17.91	BTKB
ATOM	3688	CA	MET	596	30.170	7.656	36.406	1.00	18.99	BTKB
ATOM	3689	CB	MET	596	30.204	7.773	34.877	1.00	20.77	BTKB
ATOM	3690	CG	MET	596	29.765	9.127	34.318	1.00	27.47	BTKB
ATOM	3691	SD	MET	596	28.020	9.269	33.847	1.00	36.00	BTKB
ATOM	3692	CE	MET	596	27.936	8.063	32.504	1.00	33.44	BTKB
ATOM	3693	C	MET	596	28.908	6.942	36.856	1.00	18.04	BTKB
ATOM	3694	O	MET	596	28.785	5.731	36.683	1.00	17.78	BTKB
ATOM	3695	N	PRO	597	27.968	7.677	37.469	1.00	16.14	BTKB
ATOM	3696	CD	PRO	597	28.043	9.106	37.815	1.00	17.99	BTKB
ATOM	3697	CA	PRO	597	26.712	7.101	37.947	1.00	15.23	BTKB
ATOM	3698	CB	PRO	597	26.015	8.295	38.602	1.00	15.62	BTKB
ATOM	3699	CG	PRO	597	27.134	9.181	39.007	1.00	17.68	BTKB
ATOM	3700	C	PRO	597	25.866	6.546	36.811	1.00	16.15	BTKB
ATOM	3701	O	PRO	597	25.801	7.123	35.726	1.00	17.62	BTKB
ATOM	3702	N	TYR	598	25.222	5.417	37.081	1.00	15.61	BTKB
ATOM	3703	CA	TYR	598	24.338	4.759	36.126	1.00	15.98	BTKB
ATOM	3704	CB	TYR	598	23.083	5.610	35.896	1.00	15.24	BTKB
ATOM	3705	CG	TYR	598	22.397	5.998	37.185	1.00	14.48	BTKB

	Atom Number	Atom Type	Amino Acid Residue		X	Y	Z	Occ.	Temp Factor	
ATOM	3706	CD1	TYR	598	21.945	5.028	38.073	1.00	13.82	BTKB
ATOM	3707	CE1	TYR	598	21.387	5.377	39.290	1.00	11.98	BTKB
ATOM	3708	CD2	TYR	598	22.261	7.332	37.551	1.00	14.46	BTKB
ATOM	3709	CE2	TYR	598	21.701	7.685	38.766	1.00	10.83	BTKB
ATOM	3710	CZ	TYR	598	21.267	6.704	39.629	1.00	5.19	BTKB
ATOM	3711	OH	TYR	598	20.703	7.054	40.837	1.00	8.13	BTKB
ATOM	3712	C	TYR	598	24.985	4.381	34.801	1.00	19.01	BTKB
ATOM	3713	O	TYR	598	24.347	4.425	33.757	1.00	23.02	BTKB
ATOM	3714	N	GLU	599	26.262	4.022	34.847	1.00	21.18	BTKB
ATOM	3715	CA	GLU	599	26.990	3.602	33.653	1.00	20.51	BTKB
ATOM	3716	CB	GLU	599	28.421	3.189	34.006	1.00	25.07	BTKB
ATOM	3717	CG	GLU	599	28.524	2.125	35.102	1.00	30.47	BTKB
ATOM	3718	CD	GLU	599	28.319	2.690	36.504	1.00	26.36	BTKB
ATOM	3719	OE1	GLU	599	29.312	3.160	37.099	1.00	28.29	BTKB
ATOM	3720	OE2	GLU	599	27.171	2.665	37.008	1.00	27.77	BTKB
ATOM	3721	C	GLU	599	26.245	2.417	33.071	1.00	21.77	BTKB
ATOM	3722	O	GLU	599	25.609	1.661	33.806	1.00	21.45	BTKB
ATOM	3723	N	ARG	600	26.332	2.250	31.757	1.00	24.08	BTKB
ATOM	3724	CA	ARG	600	25.637	1.164	31.062	1.00	27.74	BTKB
ATOM	3725	CB	ARG	600	25.784	-0.179	31.806	1.00	31.38	BTKB
ATOM	3726	CG	ARG	600	26.892	-1.065	31.269	1.00	33.68	BTKB
ATOM	3727	CD	ARG	600	26.456	-1.680	29.954	1.00	34.17	BTKB
ATOM	3728	NE	ARG	600	27.570	-1.896	29.039	1.00	38.49	BTKB
ATOM	3729	CZ	ARG	600	27.804	-1.145	27.968	1.00	37.73	BTKB
ATOM	3730	NH1	ARG	600	28.841	-1.413	27.179	1.00	37.45	BTKB
ATOM	3731	NH2	ARG	600	27.001	-0.123	27.685	1.00	39.50	BTKB
ATOM	3732	C	ARG	600	24.165	1.520	30.860	1.00	27.26	BTKB
ATOM	3733	O	ARG	600	23.356	0.679	30.479	1.00	25.64	BTKB
ATOM	3734	N	PHE	601	23.830	2.775	31.133	1.00	27.59	BTKB
ATOM	3735	CA	PHE	601	22.479	3.289	30.962	1.00	26.40	BTKB
ATOM	3736	CB	PHE	601	21.869	3.704	32.302	1.00	23.15	BTKB
ATOM	3737	CG	PHE	601	21.279	2.576	33.091	1.00	17.15	BTKB
ATOM	3738	CD1	PHE	601	19.961	2.190	32.887	1.00	20.02	BTKB
ATOM	3739	CD2	PHE	601	22.017	1.944	34.083	1.00	19.77	BTKB
ATOM	3740	CE1	PHE	601	19.381	1.194	33.665	1.00	17.60	BTKB
ATOM	3741	CE2	PHE	601	21.449	0.951	34.864	1.00	16.15	BTKB
ATOM	3742	CZ	PHE	601	20.126	0.575	34.655	1.00	20.16	BTKB
ATOM	3743	C	PHE	601	22.617	4.534	30.105	1.00	28.08	BTKB
ATOM	3744	O	PHE	601	23.705	5.111	30.011	1.00	28.57	BTKB
ATOM	3745	N	THR	602	21.534	4.915	29.436	1.00	30.07	BTKB
ATOM	3746	CA	THR	602	21.530	6.116	28.610	1.00	30.13	BTKB
ATOM	3747	CB	THR	602	20.733	5.924	27.293	1.00	28.51	BTKB
ATOM	3748	OG1	THR	602	19.384	5.543	27.592	1.00	27.73	BTKB
ATOM	3749	CG2	THR	602	21.379	4.867	26.417	1.00	32.12	BTKB
ATOM	3750	C	THR	602	20.820	7.140	29.476	1.00	31.17	BTKB
ATOM	3751	O	THR	602	20.274	6.785	30.524	1.00	32.73	BTKB
ATOM	3752	N	ASN	603	20.787	8.394	29.042	1.00	30.48	BTKB
ATOM	3753	CA	ASN	603	20.117	9.419	29.827	1.00	30.44	BTKB
ATOM	3754	CB	ASN	603	20.389	10.807	29.261	1.00	32.39	BTKB
ATOM	3755	CG	ASN	603	21.239	11.644	30.186	1.00	30.79	BTKB
ATOM	3756	OD1	ASN	603	21.885	11.123	31.095	1.00	31.05	BTKB
ATOM	3757	ND2	ASN	603	21.238	12.950	29.968	1.00	32.87	BTKB
ATOM	3758	C	ASN	603	18.623	9.167	29.925	1.00	29.48	BTKB
ATOM	3759	O	ASN	603	18.041	9.265	31.009	1.00	24.85	BTKB
ATOM	3760	N	SER	604	18.011	8.817	28.797	1.00	29.99	BTKB
ATOM	3761	CA	SER	604	16.578	8.537	28.755	1.00	31.56	BTKB
ATOM	3762	CB	SER	604	16.102	8.397	27.304	1.00	32.42	BTKB
ATOM	3763	OG	SER	604	16.425	9.551	26.541	1.00	31.79	BTKB

Atom Number	Atom Type	Amino Acid Residue		X	Y	Z	Occ.	Temp Factor	
ATOM 3764	C	SER	604	16.245	7.270	29.545	1.00	32.01	BTKB
ATOM 3765	O	SER	604	15.194	7.182	30.181	1.00	34.74	BTKB
ATOM 3766	N	GLU	605	17.158	6.303	29.533	1.00	31.68	BTKB
ATOM 3767	CA	GLU	605	16.954	5.052	30.252	1.00	29.12	BTKB
ATOM 3768	CB	GLU	605	17.914	3.982	29.734	1.00	30.98	BTKB
ATOM 3769	CG	GLU	605	17.561	2.565	30.172	1.00	35.34	BTKB
ATOM 3770	CD	GLU	605	18.487	1.517	29.576	1.00	36.90	BTKB
ATOM 3771	OE1	GLU	605	19.699	1.805	29.453	1.00	38.25	BTKB
ATOM 3772	OE2	GLU	605	18.005	0.412	29.231	1.00	34.49	BTKB
ATOM 3773	C	GLU	605	17.148	5.256	31.753	1.00	29.75	BTKB
ATOM 3774	O	GLU	605	16.421	4.677	32.565	1.00	32.16	BTKB
ATOM 3775	N	THR	606	18.131	6.074	32.116	1.00	26.59	BTKB
ATOM 3776	CA	THR	606	18.422	6.373	33.512	1.00	20.20	BTKB
ATOM 3777	CB	THR	606	19.691	7.243	33.621	1.00	18.39	BTKB
ATOM 3778	OG1	THR	606	20.802	6.526	33.066	1.00	16.50	BTKB
ATOM 3779	CG2	THR	606	19.987	7.603	35.079	1.00	13.19	BTKB
ATOM 3780	C	THR	606	17.233	7.103	34.139	1.00	20.29	BTKB
ATOM 3781	O	THR	606	16.828	6.813	35.274	1.00	20.04	BTKB
ATOM 3782	N	ALA	607	16.663	8.029	33.371	1.00	22.46	BTKB
ATOM 3783	CA	ALA	607	15.510	8.816	33.801	1.00	22.03	BTKB
ATOM 3784	CB	ALA	607	15.165	9.859	32.730	1.00	21.28	BTKB
ATOM 3785	C	ALA	607	14.291	7.932	34.108	1.00	21.12	BTKB
ATOM 3786	O	ALA	607	13.614	8.121	35.123	1.00	21.53	BTKB
ATOM 3787	N	GLU	608	14.036	6.950	33.247	1.00	21.20	BTKB
ATOM 3788	CA	GLU	608	12.897	6.052	33.439	1.00	22.97	BTKB
ATOM 3789	CB	GLU	608	12.661	5.208	32.176	1.00	23.32	BTKB
ATOM 3790	CG	GLU	608	11.367	4.380	32.194	1.00	27.71	BTKB
ATOM 3791	CD	GLU	608	11.607	2.865	32.186	1.00	30.68	BTKB
ATOM 3792	OE1	GLU	608	12.115	2.334	31.172	1.00	33.86	BTKB
ATOM 3793	OE2	GLU	608	11.273	2.203	33.195	1.00	29.86	BTKB
ATOM 3794	C	GLU	608	13.096	5.136	34.651	1.00	23.05	BTKB
ATOM 3795	O	GLU	608	12.171	4.902	35.445	1.00	21.90	BTKB
ATOM 3796	N	HIS	609	14.316	4.633	34.789	1.00	20.59	BTKB
ATOM 3797	CA	HIS	609	14.652	3.729	35.870	1.00	18.86	BTKB
ATOM 3798	CB	HIS	609	15.996	3.060	35.595	1.00	21.17	BTKB
ATOM 3799	CG	HIS	609	15.908	1.918	34.634	1.00	23.56	BTKB
ATOM 3800	CD2	HIS	609	15.503	0.640	34.810	1.00	28.37	BTKB
ATOM 3801	ND1	HIS	609	16.253	2.032	33.306	1.00	27.89	BTKB
ATOM 3802	CE1	HIS	609	16.064	0.872	32.702	1.00	30.83	BTKB
ATOM 3803	NE2	HIS	609	15.610	0.010	33.594	1.00	30.60	BTKB
ATOM 3804	C	HIS	609	14.602	4.306	37.281	1.00	16.90	BTKB
ATOM 3805	O	HIS	609	14.136	3.629	38.199	1.00	21.44	BTKB
ATOM 3806	N	ILE	610	15.061	5.541	37.466	1.00	15.25	BTKB
ATOM 3807	CA	ILE	610	15.039	6.149	38.795	1.00	10.99	BTKB
ATOM 3808	CB	ILE	610	15.687	7.562	38.817	1.00	10.27	BTKB
ATOM 3809	CG2	ILE	610	15.697	8.115	40.226	1.00	10.71	BTKB
ATOM 3810	CG1	ILE	610	17.131	7.499	38.329	1.00	9.01	BTKB
ATOM 3811	CD	ILE	610	17.972	6.524	39.067	1.00	13.90	BTKB
ATOM 3812	C	ILE	610	13.608	6.244	39.312	1.00	11.94	BTKB
ATOM 3813	O	ILE	610	13.335	5.926	40.462	1.00	15.24	BTKB
ATOM 3814	N	ALA	611	12.690	6.638	38.442	1.00	15.61	BTKB
ATOM 3815	CA	ALA	611	11.291	6.767	38.823	1.00	18.54	BTKB
ATOM 3816	CB	ALA	611	10.484	7.345	37.668	1.00	18.01	BTKB
ATOM 3817	C	ALA	611	10.697	5.431	39.270	1.00	21.52	BTKB
ATOM 3818	O	ALA	611	9.972	5.365	40.267	1.00	24.49	BTKB
ATOM 3819	N	GLN	612	11.023	4.366	38.546	1.00	23.83	BTKB
ATOM 3820	CA	GLN	612	10.507	3.038	38.865	1.00	22.70	BTKB
ATOM 3821	CB	GLN	612	10.736	2.091	37.691	1.00	26.14	BTKB

	Atom Number	Atom Type	Amino Acid Residue		X	Y	Z	Occ.	Temp Factor	
ATOM	3822	CG	GLN	612	10.119	2.574	36.374	1.00	29.22	BTKB
ATOM	3823	CD	GLN	612	8.597	2.714	36.418	1.00	34.44	BTKB
ATOM	3824	OE1	GLN	612	7.956	2.447	37.434	1.00	32.43	BTKB
ATOM	3825	NE2	GLN	612	8.017	3.128	35.299	1.00	33.12	BTKB
ATOM	3826	C	GLN	612	11.084	2.453	40.151	1.00	21.66	BTKB
ATOM	3827	O	GLN	612	10.501	1.541	40.741	1.00	23.34	BTKB
ATOM	3828	N	GLY	613	12.224	2.975	40.593	1.00	20.85	BTKB
ATOM	3829	CA	GLY	613	12.816	2.488	41.824	1.00	17.52	BTKB
ATOM	3830	C	GLY	613	14.300	2.188	41.764	1.00	17.19	BTKB
ATOM	3831	O	GLY	613	14.892	1.783	42.769	1.00	16.74	BTKB
ATOM	3832	N	LEU	614	14.902	2.366	40.594	1.00	14.38	BTKB
ATOM	3833	CA	LEU	614	16.327	2.105	40.427	1.00	13.63	BTKB
ATOM	3834	CB	LEU	614	16.701	2.152	38.947	1.00	11.11	BTKB
ATOM	3835	CG	LEU	614	18.127	1.939	38.433	1.00	10.02	BTKB
ATOM	3836	CD1	LEU	614	18.886	3.239	38.427	1.00	8.37	BTKB
ATOM	3837	CD2	LEU	614	18.842	0.853	39.211	1.00	13.13	BTKB
ATOM	3838	C	LEU	614	17.183	3.065	41.248	1.00	13.27	BTKB
ATOM	3839	O	LEU	614	16.938	4.274	41.278	1.00	11.31	BTKB
ATOM	3840	N	ARG	615	18.206	2.502	41.889	1.00	13.39	BTKB
ATOM	3841	CA	ARG	615	19.130	3.240	42.735	1.00	11.32	BTKB
ATOM	3842	CB	ARG	615	18.781	3.016	44.206	1.00	13.75	BTKB
ATOM	3843	CG	ARG	615	17.381	3.443	44.614	1.00	14.44	BTKB
ATOM	3844	CD	ARG	615	17.228	4.946	44.642	1.00	12.94	BTKB
ATOM	3845	NE	ARG	615	15.899	5.303	45.124	1.00	11.71	BTKB
ATOM	3846	CZ	ARG	615	14.893	5.685	44.345	1.00	11.61	BTKB
ATOM	3847	NH1	ARG	615	15.058	5.772	43.036	1.00	13.30	BTKB
ATOM	3848	NH2	ARG	615	13.708	5.949	44.876	1.00	16.80	BTKB
ATOM	3849	C	ARG	615	20.564	2.773	42.501	1.00	12.33	BTKB
ATOM	3850	O	ARG	615	20.807	1.751	41.850	1.00	14.35	BTKB
ATOM	3851	N	LEU	616	21.504	3.526	43.066	1.00	17.12	BTKB
ATOM	3852	CA	LEU	616	22.936	3.251	42.967	1.00	13.55	BTKB
ATOM	3853	CB	LEU	616	23.730	4.525	43.258	1.00	12.49	BTKB
ATOM	3854	CG	LEU	616	24.452	5.273	42.132	1.00	15.47	BTKB
ATOM	3855	CD1	LEU	616	24.288	4.570	40.788	1.00	20.12	BTKB
ATOM	3856	CD2	LEU	616	23.990	6.720	42.086	1.00	11.52	BTKB
ATOM	3857	C	LEU	616	23.337	2.177	43.961	1.00	12.84	BTKB
ATOM	3858	O	LEU	616	22.963	2.234	45.135	1.00	11.91	BTKB
ATOM	3859	N	TYR	617	24.100	1.200	43.483	1.00	12.87	BTKB
ATOM	3860	CA	TYR	617	24.561	0.109	44.322	1.00	8.22	BTKB
ATOM	3861	CB	TYR	617	25.037	-1.067	43.453	1.00	7.64	BTKB
ATOM	3862	CG	TYR	617	26.116	-0.724	42.444	1.00	4.38	BTKB
ATOM	3863	CD1	TYR	617	27.400	-0.394	42.852	1.00	5.18	BTKB
ATOM	3864	CE1	TYR	617	28.382	-0.065	41.935	1.00	5.80	BTKB
ATOM	3865	CD2	TYR	617	25.843	-0.722	41.082	1.00	6.41	BTKB
ATOM	3866	CE2	TYR	617	26.827	-0.395	40.148	1.00	7.22	BTKB
ATOM	3867	CZ	TYR	617	28.092	-0.070	40.584	1.00	7.64	BTKB
ATOM	3868	OH	TYR	617	29.082	0.223	39.674	1.00	9.96	BTKB
ATOM	3869	C	TYR	617	25.679	0.600	45.239	1.00	8.77	BTKB
ATOM	3870	O	TYR	617	26.286	1.631	44.990	1.00	7.36	BTKB
ATOM	3871	N	ARG	618	25.952	-0.147	46.295	1.00	8.18	BTKB
ATOM	3872	CA	ARG	618	27.001	0.219	47.229	1.00	8.36	BTKB
ATOM	3873	CB	ARG	618	26.879	-0.618	48.511	1.00	6.48	BTKB
ATOM	3874	CG	ARG	618	27.967	-0.360	49.527	1.00	6.90	BTKB
ATOM	3875	CD	ARG	618	27.593	-0.867	50.907	1.00	9.82	BTKB
ATOM	3876	NE	ARG	618	27.871	-2.281	51.118	1.00	14.88	BTKB
ATOM	3877	CZ	ARG	618	28.894	-2.735	51.835	1.00	13.15	BTKB
ATOM	3878	NH1	ARG	618	29.733	-1.888	52.394	1.00	14.59	BTKB
ATOM	3879	NH2	ARG	618	29.052	-4.033	52.047	1.00	13.61	BTKB

	Atom Number	Atom Type	Amino Acid Residue		X	Y	Z	Occ.	Temp Factor	
ATOM	3880	C	ARG	618	28.383	0.013	46.616	1.00	8.62	BTKB
ATOM	3881	O	ARG	618	28.688	-1.062	46.086	1.00	10.77	BTKB
ATOM	3882	N	PRO	619	29.220	1.057	46.623	1.00	6.53	BTKB
ATOM	3883	CD	PRO	619	28.936	2.487	46.840	1.00	3.47	BTKB
ATOM	3884	CA	PRO	619	30.553	0.869	46.051	1.00	8.75	BTKB
ATOM	3885	CB	PRO	619	31.116	2.286	46.032	1.00	5.78	BTKB
ATOM	3886	CG	PRO	619	29.882	3.142	45.874	1.00	5.70	BTKB
ATOM	3887	C	PRO	619	31.382	-0.040	46.962	1.00	11.49	BTKB
ATOM	3888	O	PRO	619	31.251	-0.002	48.188	1.00	8.13	BTKB
ATOM	3889	N	HIS	620	32.192	-0.896	46.351	1.00	13.39	BTKB
ATOM	3890	CA	HIS	620	33.058	-1.805	47.090	1.00	16.43	BTKB
ATOM	3891	CB	HIS	620	34.061	-2.507	46.145	1.00	23.71	BTKB
ATOM	3892	CG	HIS	620	34.288	-1.798	44.833	1.00	29.79	BTKB
ATOM	3893	CD2	HIS	620	34.138	-0.503	44.468	1.00	31.60	BTKB
ATOM	3894	ND1	HIS	620	34.719	-2.464	43.704	1.00	31.86	BTKB
ATOM	3895	CE1	HIS	620	34.820	-1.607	42.699	1.00	33.57	BTKB
ATOM	3896	NE2	HIS	620	34.471	-0.411	43.140	1.00	35.83	BTKB
ATOM	3897	C	HIS	620	33.804	-1.148	48.267	1.00	15.65	BTKB
ATOM	3898	O	HIS	620	33.963	-1.764	49.328	1.00	14.45	BTKB
ATOM	3899	N	LEU	621	34.235	0.100	48.080	1.00	11.67	BTKB
ATOM	3900	CA	LEU	621	34.974	0.834	49.103	1.00	9.74	BTKB
ATOM	3901	CB	LEU	621	35.792	1.955	48.464	1.00	12.10	BTKB
ATOM	3902	CG	LEU	621	36.869	1.540	47.459	1.00	10.83	BTKB
ATOM	3903	CD1	LEU	621	36.318	1.644	46.047	1.00	12.43	BTKB
ATOM	3904	CD2	LEU	621	38.078	2.426	47.601	1.00	13.18	BTKB
ATOM	3905	C	LEU	621	34.155	1.404	50.261	1.00	10.03	BTKB
ATOM	3906	O	LEU	621	34.717	1.801	51.284	1.00	10.92	BTKB
ATOM	3907	N	ALA	622	32.836	1.436	50.101	1.00	10.32	BTKB
ATOM	3908	CA	ALA	622	31.944	1.964	51.120	1.00	11.25	BTKB
ATOM	3909	CB	ALA	622	30.700	2.563	50.460	1.00	12.08	BTKB
ATOM	3910	C	ALA	622	31.536	0.862	52.085	1.00	13.04	BTKB
ATOM	3911	O	ALA	622	31.502	-0.307	51.719	1.00	15.23	BTKB
ATOM	3912	N	SER	623	31.279	1.230	53.332	1.00	14.15	BTKB
ATOM	3913	CA	SER	623	30.837	0.270	54.325	1.00	11.19	BTKB
ATOM	3914	CB	SER	623	31.416	0.611	55.696	1.00	9.54	BTKB
ATOM	3915	OG	SER	623	30.949	1.864	56.170	1.00	8.50	BTKB
ATOM	3916	C	SER	623	29.312	0.331	54.349	1.00	10.40	BTKB
ATOM	3917	O	SER	623	28.702	1.234	53.768	1.00	14.47	BTKB
ATOM	3918	N	GLU	624	28.692	-0.651	54.985	1.00	10.03	BTKB
ATOM	3919	CA	GLU	624	27.238	-0.714	55.093	1.00	10.70	BTKB
ATOM	3920	CB	GLU	624	26.869	-1.867	56.027	1.00	15.43	BTKB
ATOM	3921	CG	GLU	624	25.423	-1.946	56.491	1.00	15.78	BTKB
ATOM	3922	CD	GLU	624	25.244	-2.977	57.601	1.00	19.80	BTKB
ATOM	3923	OE1	GLU	624	26.105	-3.060	58.503	1.00	22.20	BTKB
ATOM	3924	OE2	GLU	624	24.240	-3.709	57.574	1.00	22.73	BTKB
ATOM	3925	C	GLU	624	26.660	0.605	55.612	1.00	10.33	BTKB
ATOM	3926	O	GLU	624	25.627	1.078	55.124	1.00	12.18	BTKB
ATOM	3927	N	LYS	625	27.335	1.202	56.591	1.00	13.68	BTKB
ATOM	3928	CA	LYS	625	26.886	2.461	57.172	1.00	13.17	BTKB
ATOM	3929	CB	LYS	625	27.641	2.761	58.470	1.00	13.89	BTKB
ATOM	3930	CG	LYS	625	26.960	3.806	59.351	1.00	19.82	BTKB
ATOM	3931	CD	LYS	625	27.145	3.522	60.843	1.00	21.52	BTKB
ATOM	3932	CE	LYS	625	26.398	2.261	61.281	1.00	24.13	BTKB
ATOM	3933	NZ	LYS	625	26.554	1.946	62.735	1.00	26.73	BTKB
ATOM	3934	C	LYS	625	27.007	3.608	56.175	1.00	12.94	BTKB
ATOM	3935	O	LYS	625	26.074	4.393	56.023	1.00	17.08	BTKB
ATOM	3936	N	VAL	626	28.118	3.671	55.446	1.00	13.16	BTKB
ATOM	3937	CA	VAL	626	28.310	4.726	54.445	1.00	10.56	BTKB

	Atom Number	Atom Type	Amino Acid Residue		X	Y	Z	Occ.	Temp Factor	
ATOM	3938	CB	VAL	626	29.698	4.646	53.758	1.00	10.58	BTKB
ATOM	3939	CG1	VAL	626	29.775	5.671	52.634	1.00	13.96	BTKB
ATOM	3940	CG2	VAL	626	30.802	4.904	54.763	1.00	6.81	BTKB
ATOM	3941	C	VAL	626	27.221	4.653	53.368	1.00	8.76	BTKB
ATOM	3942	O	VAL	626	26.757	5.681	52.870	1.00	6.95	BTKB
ATOM	3943	N	TYR	627	26.827	3.438	53.001	1.00	7.31	BTKB
ATOM	3944	CA	TYR	627	25.780	3.243	52.001	1.00	7.99	BTKB
ATOM	3945	CB	TYR	627	25.674	1.773	51.598	1.00	2.15	BTKB
ATOM	3946	CG	TYR	627	24.723	1.544	50.454	1.00	4.61	BTKB
ATOM	3947	CD1	TYR	627	24.718	2.400	49.352	1.00	10.72	BTKB
ATOM	3948	CE1	TYR	627	23.845	2.201	48.298	1.00	9.43	BTKB
ATOM	3949	CD2	TYR	627	23.828	0.482	50.468	1.00	5.07	BTKB
ATOM	3950	CE2	TYR	627	22.946	0.273	49.410	1.00	6.61	BTKB
ATOM	3951	CZ	TYR	627	22.962	1.139	48.334	1.00	5.55	BTKB
ATOM	3952	OH	TYR	627	22.092	0.961	47.297	1.00	11.16	BTKB
ATOM	3953	C	TYR	627	24.429	3.715	52.518	1.00	9.39	BTKB
ATOM	3954	O	TYR	627	23.599	4.187	51.754	1.00	11.16	BTKB
ATOM	3955	N	THR	628	24.201	3.546	53.813	1.00	9.89	BTKB
ATOM	3956	CA	THR	628	22.961	3.976	54.447	1.00	9.04	BTKB
ATOM	3957	CB	THR	628	22.989	3.636	55.961	1.00	10.10	BTKB
ATOM	3958	OG1	THR	628	23.201	2.229	56.132	1.00	13.62	BTKB
ATOM	3959	CG2	THR	628	21.691	4.033	56.633	1.00	6.51	BTKB
ATOM	3960	C	THR	628	22.868	5.490	54.289	1.00	7.33	BTKB
ATOM	3961	O	THR	628	21.856	6.023	53.853	1.00	6.66	BTKB
ATOM	3962	N	ILE	629	23.967	6.167	54.589	1.00	6.78	BTKB
ATOM	3963	CA	ILE	629	24.031	7.617	54.493	1.00	8.03	BTKB
ATOM	3964	CB	ILE	629	25.417	8.151	54.964	1.00	6.17	BTKB
ATOM	3965	CG2	ILE	629	25.531	9.649	54.709	1.00	5.05	BTKB
ATOM	3966	CG1	ILE	629	25.593	7.854	56.459	1.00	5.15	BTKB
ATOM	3967	CD	ILE	629	26.999	8.035	56.969	1.00	2.34	BTKB
ATOM	3968	C	ILE	629	23.690	8.120	53.085	1.00	12.02	BTKB
ATOM	3969	O	ILE	629	22.702	8.842	52.900	1.00	13.66	BTKB
ATOM	3970	N	MET	630	24.439	7.676	52.085	1.00	11.42	BTKB
ATOM	3971	CA	MET	630	24.185	8.124	50.727	1.00	7.89	BTKB
ATOM	3972	CB	MET	630	25.249	7.600	49.756	1.00	11.44	BTKB
ATOM	3973	CG	MET	630	25.288	6.095	49.574	1.00	14.27	BTKB
ATOM	3974	SD	MET	630	26.438	5.613	48.277	1.00	14.21	BTKB
ATOM	3975	CE	MET	630	27.987	5.700	49.104	1.00	3.93	BTKB
ATOM	3976	C	MET	630	22.798	7.766	50.246	1.00	6.76	BTKB
ATOM	3977	O	MET	630	22.164	8.542	49.525	1.00	9.02	BTKB
ATOM	3978	N	TYR	631	22.303	6.618	50.696	1.00	9.53	BTKB
ATOM	3979	CA	TYR	631	20.981	6.143	50.301	1.00	9.62	BTKB
ATOM	3980	CB	TYR	631	20.837	4.637	50.583	1.00	7.23	BTKB
ATOM	3981	CG	TYR	631	19.708	3.978	49.819	1.00	9.49	BTKB
ATOM	3982	CD1	TYR	631	18.385	4.120	50.232	1.00	12.76	BTKB
ATOM	3983	CE1	TYR	631	17.343	3.539	49.518	1.00	12.89	BTKB
ATOM	3984	CD2	TYR	631	19.962	3.233	48.670	1.00	8.23	BTKB
ATOM	3985	CE2	TYR	631	18.929	2.646	47.951	1.00	11.55	BTKB
ATOM	3986	CZ	TYR	631	17.625	2.803	48.381	1.00	13.98	BTKB
ATOM	3987	OH	TYR	631	16.598	2.225	47.683	1.00	16.12	BTKB
ATOM	3988	C	TYR	631	19.844	6.937	50.950	1.00	7.30	BTKB
ATOM	3989	O	TYR	631	18.719	6.932	50.451	1.00	11.12	BTKB
ATOM	3990	N	SER	632	20.119	7.635	52.048	1.00	9.61	BTKB
ATOM	3991	CA	SER	632	19.067	8.423	52.678	1.00	9.92	BTKB
ATOM	3992	CB	SER	632	19.446	8.838	54.108	1.00	7.09	BTKB
ATOM	3993	OG	SER	632	20.592	9.664	54.130	1.00	8.65	BTKB
ATOM	3994	C	SER	632	18.759	9.642	51.800	1.00	10.16	BTKB
ATOM	3995	O	SER	632	17.648	10.189	51.820	1.00	8.62	BTKB

	Atom Number	Atom Type	Amino Acid Residue		X	Y	Z	Occ.	Temp Factor	
ATOM	3996	N	CYS	633	19.734	10.013	50.979	1.00	13.59	BTKB
ATOM	3997	CA	CYS	633	19.606	11.146	50.065	1.00	13.01	BTKB
ATOM	3998	CB	CYS	633	20.988	11.537	49.522	1.00	9.51	BTKB
ATOM	3999	SG	CYS	633	22.269	11.873	50.748	1.00	10.09	BTKB
ATOM	4000	C	CYS	633	18.688	10.861	48.869	1.00	11.24	BTKB
ATOM	4001	O	CYS	633	18.167	11.785	48.264	1.00	11.58	BTKB
ATOM	4002	N	TRP	634	18.448	9.590	48.565	1.00	12.35	BTKB
ATOM	4003	CA	TRP	634	17.649	9.225	47.396	1.00	16.45	BTKB
ATOM	4004	CB	TRP	634	18.354	8.109	46.629	1.00	14.41	BTKB
ATOM	4005	CG	TRP	634	19.803	8.397	46.406	1.00	16.37	BTKB
ATOM	4006	CD2	TRP	634	20.885	7.465	46.489	1.00	13.01	BTKB
ATOM	4007	CE2	TRP	634	22.067	8.178	46.219	1.00	13.10	BTKB
ATOM	4008	CE3	TRP	634	20.965	6.095	46.765	1.00	12.84	BTKB
ATOM	4009	CD1	TRP	634	20.361	9.604	46.101	1.00	12.67	BTKB
ATOM	4010	NE1	TRP	634	21.717	9.482	45.987	1.00	11.33	BTKB
ATOM	4011	CZ2	TRP	634	23.325	7.566	46.214	1.00	10.17	BTKB
ATOM	4012	CZ3	TRP	634	22.213	5.490	46.761	1.00	12.02	BTKB
ATOM	4013	CH2	TRP	634	23.376	6.227	46.486	1.00	4.94	BTKB
ATOM	4014	C	TRP	634	16.171	8.881	47.541	1.00	20.48	BTKB
ATOM	4015	O	TRP	634	15.588	8.288	46.633	1.00	24.09	BTKB
ATOM	4016	N	HIS	635	15.550	9.253	48.654	1.00	22.92	BTKB
ATOM	4017	CA	HIS	635	14.128	8.968	48.833	1.00	24.53	BTKB
ATOM	4018	CB	HIS	635	13.670	9.356	50.234	1.00	25.26	BTKB
ATOM	4019	CG	HIS	635	14.517	8.796	51.331	1.00	34.35	BTKB
ATOM	4020	CD2	HIS	635	14.645	9.161	52.628	1.00	37.85	BTKB
ATOM	4021	ND1	HIS	635	15.373	7.731	51.144	1.00	40.01	BTKB
ATOM	4022	CE1	HIS	635	15.990	7.465	52.282	1.00	41.13	BTKB
ATOM	4023	NE2	HIS	635	15.567	8.319	53.198	1.00	40.19	BTKB
ATOM	4024	C	HIS	635	13.361	9.805	47.810	1.00	24.66	BTKB
ATOM	4025	O	HIS	635	13.551	11.016	47.734	1.00	23.32	BTKB
ATOM	4026	N	GLU	636	12.488	9.179	47.031	1.00	26.44	BTKB
ATOM	4027	CA	GLU	636	11.734	9.939	46.043	1.00	26.89	BTKB
ATOM	4028	CB	GLU	636	10.949	9.006	45.110	1.00	28.33	BTKB
ATOM	4029	CG	GLU	636	10.700	9.603	43.709	1.00	28.10	BTKB
ATOM	4030	CD	GLU	636	10.649	8.559	42.592	1.00	22.86	BTKB
ATOM	4031	OE1	GLU	636	9.696	8.602	41.786	1.00	21.50	BTKB
ATOM	4032	OE2	GLU	636	11.572	7.715	42.501	1.00	21.58	BTKB
ATOM	4033	C	GLU	636	10.831	10.959	46.753	1.00	27.63	BTKB
ATOM	4034	O	GLU	636	10.420	11.954	46.156	1.00	30.62	BTKB
ATOM	4035	N	LYS	637	10.529	10.714	48.026	1.00	25.98	BTKB
ATOM	4036	CA	LYS	637	9.724	11.642	48.817	1.00	26.32	BTKB
ATOM	4037	CB	LYS	637	8.924	10.898	49.896	1.00	28.32	BTKB
ATOM	4038	CG	LYS	637	8.125	11.800	50.857	1.00	29.37	BTKB
ATOM	4039	CD	LYS	637	6.661	11.997	50.426	1.00	31.37	BTKB
ATOM	4040	CE	LYS	637	6.512	12.837	49.155	1.00	33.19	BTKB
ATOM	4041	NZ	LYS	637	5.123	12.793	48.607	1.00	32.03	BTKB
ATOM	4042	C	LYS	637	10.701	12.606	49.485	1.00	26.98	BTKB
ATOM	4043	O	LYS	637	11.212	12.330	50.575	1.00	26.07	BTKB
ATOM	4044	N	ALA	638	10.960	13.729	48.825	1.00	28.49	BTKB
ATOM	4045	CA	ALA	638	11.879	14.746	49.333	1.00	28.72	BTKB
ATOM	4046	CB	ALA	638	11.658	16.048	48.586	1.00	31.16	BTKB
ATOM	4047	C	ALA	638	11.779	14.985	50.844	1.00	28.22	BTKB
ATOM	4048	O	ALA	638	12.791	15.134	51.529	1.00	25.48	BTKB
ATOM	4049	N	ASP	639	10.554	15.003	51.355	1.00	29.23	BTKB
ATOM	4050	CA	ASP	639	10.295	15.234	52.774	1.00	28.43	BTKB
ATOM	4051	CB	ASP	639	8.779	15.248	53.031	1.00	31.75	BTKB
ATOM	4052	CG	ASP	639	8.058	16.380	52.288	1.00	34.13	BTKB
ATOM	4053	OD1	ASP	639	6.951	16.765	52.735	1.00	33.09	BTKB

	Atom Number	Atom Type	Amino Acid Residue		X	Y	Z	Occ.	Temp Factor	
ATOM	4054	OD2	ASP	639	8.586	16.881	51.266	1.00	36.59	BTKB
ATOM	4055	C	ASP	639	10.970	14.230	53.718	1.00	28.45	BTKB
ATOM	4056	O	ASP	639	11.329	14.574	54.848	1.00	25.09	BTKB
ATOM	4057	N	GLU	640	11.146	12.996	53.244	1.00	24.72	BTKB
ATOM	4058	CA	GLU	640	11.754	11.931	54.038	1.00	18.61	BTKB
ATOM	4059	CB	GLU	640	11.297	10.563	53.513	1.00	20.35	BTKB
ATOM	4060	CG	GLU	640	11.609	9.361	54.422	1.00	22.93	BTKB
ATOM	4061	CD	GLU	640	11.329	8.007	53.762	1.00	21.79	BTKB
ATOM	4062	OE1	GLU	640	10.997	7.043	54.486	1.00	26.11	BTKB
ATOM	4063	OE2	GLU	640	11.465	7.895	52.522	1.00	15.76	BTKB
ATOM	4064	C	GLU	640	13.276	12.021	54.030	1.00	18.11	BTKB
ATOM	4065	O	GLU	640	13.950	11.266	54.734	1.00	19.30	BTKB
ATOM	4066	N	ARG	641	13.821	12.935	53.233	1.00	16.37	BTKB
ATOM	4067	CA	ARG	641	15.273	13.108	53.155	1.00	14.52	BTKB
ATOM	4068	CB	ARG	641	15.682	13.695	51.803	1.00	12.65	BTKB
ATOM	4069	CG	ARG	641	15.358	12.831	50.610	1.00	8.88	BTKB
ATOM	4070	CD	ARG	641	15.886	13.474	49.360	1.00	11.30	BTKB
ATOM	4071	NE	ARG	641	15.231	12.947	48.171	1.00	11.72	BTKB
ATOM	4072	CZ	ARG	641	14.731	13.710	47.206	1.00	13.82	BTKB
ATOM	4073	NH1	ARG	641	14.827	15.031	47.288	1.00	12.20	BTKB
ATOM	4074	NH2	ARG	641	14.071	13.160	46.198	1.00	16.65	BTKB
ATOM	4075	C	ARG	641	15.825	13.988	54.279	1.00	14.27	BTKB
ATOM	4076	O	ARG	641	15.198	14.964	54.692	1.00	16.92	BTKB
ATOM	4077	N	PRO	642	17.017	13.642	54.787	1.00	11.73	BTKB
ATOM	4078	CD	PRO	642	17.769	12.438	54.386	1.00	8.97	BTKB
ATOM	4079	CA	PRO	642	17.706	14.357	55.863	1.00	11.49	BTKB
ATOM	4080	CB	PRO	642	18.793	13.371	56.269	1.00	10.83	BTKB
ATOM	4081	CG	PRO	642	19.134	12.705	54.949	1.00	11.19	BTKB
ATOM	4082	C	PRO	642	18.313	15.686	55.423	1.00	12.59	BTKB
ATOM	4083	O	PRO	642	18.396	15.982	54.235	1.00	14.26	BTKB
ATOM	4084	N	THR	643	18.687	16.513	56.391	1.00	13.95	BTKB
ATOM	4085	CA	THR	643	19.310	17.790	56.081	1.00	11.71	BTKB
ATOM	4086	CB	THR	643	19.003	18.856	57.151	1.00	9.31	BTKB
ATOM	4087	OG1	THR	643	19.178	18.295	58.453	1.00	13.11	BTKB
ATOM	4088	CG2	THR	643	17.585	19.370	57.013	1.00	16.43	BTKB
ATOM	4089	C	THR	643	20.815	17.574	56.032	1.00	9.69	BTKB
ATOM	4090	O	THR	643	21.310	16.524	56.455	1.00	10.98	BTKB
ATOM	4091	N	PHE	644	21.542	18.544	55.489	1.00	8.04	BTKB
ATOM	4092	CA	PHE	644	22.994	18.461	55.430	1.00	7.60	BTKB
ATOM	4093	CB	PHE	644	23.564	19.613	54.593	1.00	9.27	BTKB
ATOM	4094	CG	PHE	644	23.518	19.373	53.106	1.00	11.88	BTKB
ATOM	4095	CD1	PHE	644	24.271	18.353	52.530	1.00	10.79	BTKB
ATOM	4096	CD2	PHE	644	22.749	20.185	52.275	1.00	17.35	BTKB
ATOM	4097	CE1	PHE	644	24.262	18.145	51.147	1.00	15.55	BTKB
ATOM	4098	CE2	PHE	644	22.733	19.984	50.885	1.00	14.48	BTKB
ATOM	4099	CZ	PHE	644	23.495	18.959	50.324	1.00	11.64	BTKB
ATOM	4100	C	PHE	644	23.524	18.508	56.866	1.00	8.95	BTKB
ATOM	4101	O	PHE	644	24.601	17.996	57.163	1.00	10.35	BTKB
ATOM	4102	N	LYS	645	22.736	19.096	57.760	1.00	10.75	BTKB
ATOM	4103	CA	LYS	645	23.098	19.189	59.168	1.00	14.25	BTKB
ATOM	4104	CB	LYS	645	22.094	20.076	59.914	1.00	20.40	BTKB
ATOM	4105	CG	LYS	645	22.396	20.305	61.404	1.00	19.51	BTKB
ATOM	4106	CD	LYS	645	23.765	20.942	61.644	1.00	21.82	BTKB
ATOM	4107	CE	LYS	645	24.857	19.891	61.826	1.00	18.46	BTKB
ATOM	4108	NZ	LYS	645	26.212	20.491	61.891	1.00	19.87	BTKB
ATOM	4109	C	LYS	645	23.121	17.795	59.784	1.00	12.92	BTKB
ATOM	4110	O	LYS	645	24.061	17.433	60.491	1.00	16.72	BTKB
ATOM	4111	N	ILE	646	22.067	17.027	59.528	1.00	12.66	BTKB

	Atom Number	Atom Type	Amino Acid Residue		X	Y	Z	Occ.	Temp Factor	
ATOM	4112	CA	ILE	646	21.949	15.658	60.026	1.00	12.65	BTKB
ATOM	4113	CB	ILE	646	20.527	15.115	59.763	1.00	16.20	BTKB
ATOM	4114	CG2	ILE	646	20.494	13.594	59.881	1.00	18.66	BTKB
ATOM	4115	CG1	ILE	646	19.536	15.781	60.726	1.00	16.13	BTKB
ATOM	4116	CD	ILE	646	18.071	15.534	60.391	1.00	16.31	BTKB
ATOM	4117	C	ILE	646	22.996	14.806	59.305	1.00	14.43	BTKB
ATOM	4118	O	ILE	646	23.772	14.089	59.946	1.00	13.14	BTKB
ATOM	4119	N	LEU	647	23.054	14.957	57.979	1.00	14.30	BTKB
ATOM	4120	CA	LEU	647	24.006	14.254	57.113	1.00	14.73	BTKB
ATOM	4121	CB	LEU	647	23.879	14.795	55.682	1.00	16.19	BTKB
ATOM	4122	CG	LEU	647	23.584	13.896	54.473	1.00	13.29	BTKB
ATOM	4123	CD1	LEU	647	22.737	12.680	54.829	1.00	12.13	BTKB
ATOM	4124	CD2	LEU	647	22.884	14.734	53.433	1.00	9.14	BTKB
ATOM	4125	C	LEU	647	25.427	14.468	57.633	1.00	12.35	BTKB
ATOM	4126	O	LEU	647	26.247	13.556	57.613	1.00	10.67	BTKB
ATOM	4127	N	LEU	648	25.692	15.666	58.142	1.00	11.64	BTKB
ATOM	4128	CA	LEU	648	26.996	15.998	58.702	1.00	12.42	BTKB
ATOM	4129	CB	LEU	648	27.125	17.515	58.914	1.00	9.53	BTKB
ATOM	4130	CG	LEU	648	28.505	18.085	59.272	1.00	10.27	BTKB
ATOM	4131	CD1	LEU	648	29.570	17.603	58.313	1.00	9.87	BTKB
ATOM	4132	CD2	LEU	648	28.441	19.577	59.254	1.00	7.44	BTKB
ATOM	4133	C	LEU	648	27.269	15.241	60.009	1.00	13.83	BTKB
ATOM	4134	O	LEU	648	28.369	14.729	60.210	1.00	12.04	BTKB
ATOM	4135	N	SER	649	26.271	15.152	60.886	1.00	13.67	BTKB
ATOM	4136	CA	SER	649	26.439	14.440	62.158	1.00	11.87	BTKB
ATOM	4137	CB	SER	649	25.187	14.575	63.035	1.00	10.55	BTKB
ATOM	4138	OG	SER	649	24.887	15.929	63.307	1.00	12.87	BTKB
ATOM	4139	C	SER	649	26.711	12.958	61.910	1.00	11.53	BTKB
ATOM	4140	O	SER	649	27.719	12.413	62.366	1.00	14.67	BTKB
ATOM	4141	N	ASN	650	25.808	12.317	61.175	1.00	12.17	BTKB
ATOM	4142	CA	ASN	650	25.918	10.897	60.849	1.00	10.92	BTKB
ATOM	4143	CB	ASN	650	24.804	10.487	59.880	1.00	11.30	BTKB
ATOM	4144	CG	ASN	650	23.414	10.618	60.498	1.00	14.31	BTKB
ATOM	4145	OD1	ASN	650	23.236	11.298	61.506	1.00	16.85	BTKB
ATOM	4146	ND2	ASN	650	22.429	9.962	59.902	1.00	15.42	BTKB
ATOM	4147	C	ASN	650	27.280	10.549	60.272	1.00	11.25	BTKB
ATOM	4148	O	ASN	650	27.843	9.516	60.592	1.00	11.41	BTKB
ATOM	4149	N	ILE	651	27.809	11.425	59.425	1.00	11.24	BTKB
ATOM	4150	CA	ILE	651	29.119	11.227	58.823	1.00	11.82	BTKB
ATOM	4151	CB	ILE	651	29.364	12.262	57.707	1.00	10.65	BTKB
ATOM	4152	CG2	ILE	651	30.825	12.736	57.688	1.00	13.31	BTKB
ATOM	4153	CG1	ILE	651	28.933	11.679	56.358	1.00	9.82	BTKB
ATOM	4154	CD	ILE	651	28.910	12.690	55.219	1.00	9.11	BTKB
ATOM	4155	C	ILE	651	30.214	11.306	59.884	1.00	15.31	BTKB
ATOM	4156	O	ILE	651	31.166	10.527	59.854	1.00	17.19	BTKB
ATOM	4157	N	LEU	652	30.069	12.230	60.831	1.00	17.10	BTKB
ATOM	4158	CA	LEU	652	31.059	12.394	61.888	1.00	14.72	BTKB
ATOM	4159	CB	LEU	652	30.796	13.654	62.717	1.00	13.15	BTKB
ATOM	4160	CG	LEU	652	31.745	14.827	62.444	1.00	8.61	BTKB
ATOM	4161	CD1	LEU	652	32.998	14.338	61.694	1.00	10.58	BTKB
ATOM	4162	CD2	LEU	652	31.041	15.927	61.663	1.00	9.95	BTKB
ATOM	4163	C	LEU	652	31.233	11.180	62.790	1.00	16.01	BTKB
ATOM	4164	O	LEU	652	32.285	11.022	63.398	1.00	16.51	BTKB
ATOM	4165	N	ASP	653	30.209	10.345	62.920	1.00	21.54	BTKB
ATOM	4166	CA	ASP	653	30.356	9.145	63.732	1.00	24.79	BTKB
ATOM	4167	CB	ASP	653	29.651	9.264	65.099	1.00	28.24	BTKB
ATOM	4168	CG	ASP	653	28.171	9.543	64.990	1.00	24.00	BTKB
ATOM	4169	OD1	ASP	653	27.389	8.597	64.778	1.00	22.42	BTKB

	Atom Number	Atom Type	Amino Acid Residue		X	Y	Z	Occ.	Temp Factor	
ATOM	4170	OD2	ASP	653	27.780	10.711	65.170	1.00	31.86	BTKB
ATOM	4171	C	ASP	653	29.989	7.854	62.996	1.00	29.44	BTKB
ATOM	4172	O	ASP	653	28.983	7.207	63.287	1.00	31.02	BTKB
ATOM	4173	N	VAL	654	30.804	7.508	62.006	1.00	33.61	BTKB
ATOM	4174	CA	VAL	654	30.603	6.289	61.233	1.00	34.38	BTKB
ATOM	4175	CB	VAL	654	30.615	6.548	59.700	1.00	33.33	BTKB
ATOM	4176	CG1	VAL	654	30.247	5.284	58.958	1.00	31.87	BTKB
ATOM	4177	CG2	VAL	654	29.668	7.660	59.331	1.00	28.22	BTKB
ATOM	4178	C	VAL	654	31.766	5.368	61.580	1.00	37.78	BTKB
ATOM	4179	OT1	VAL	654	31.521	4.332	62.236	1.00	39.69	BTKB
ATOM	4180	OT2	VAL	654	32.916	5.722	61.230	1.00	36.40	BTKB
END										

ABSTRACT

The invention provides crystal structure of the kinase domain of BTK, as well as use of the crystal structure in the design, identification, and verification of ligands that modulate BTK activity.

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